



What have urban experiments taught us about atmospheric flow and transport?

Urban Flow and Transport Model Development and Evaluation with Field Experiments

Julie K. Lundquist

Stevens T. Chan, Branko Kosović, Fotini K. Chow*

National Atmospheric Release Advisory Center

Energy & Environment Directorate

Lawrence Livermore National Laboratory, Livermore, CA

***now at University of California at Berkeley**

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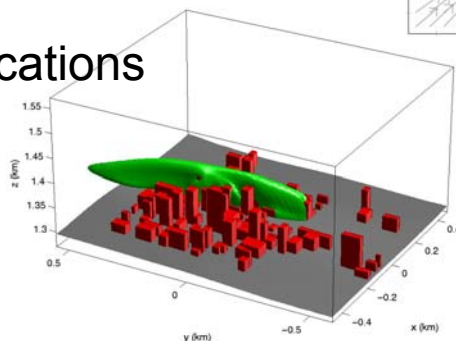
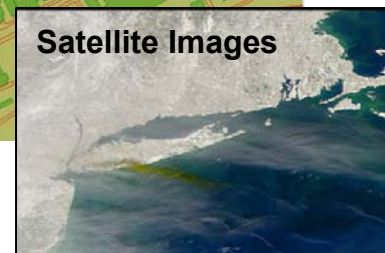
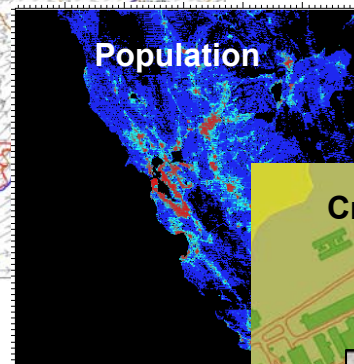
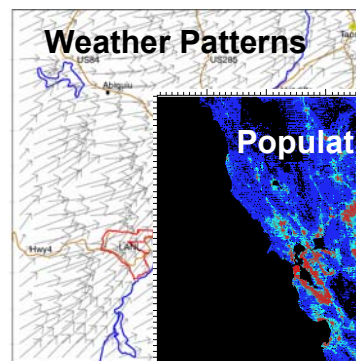
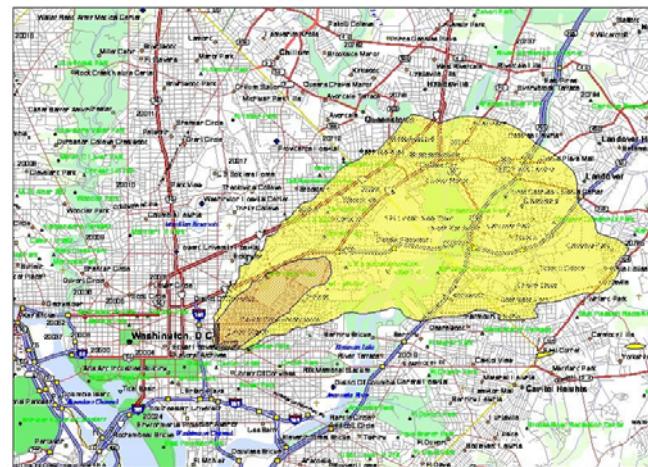
Presentation to California Air Resources Board

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The Department of Homeland Security sponsored the production of this material under the Department of Energy contract for the management and operation of Lawrence Livermore National Laboratory

LLNL develops and operationalizes tools for high-resolution prediction of atmospheric flow, transport, and dispersion



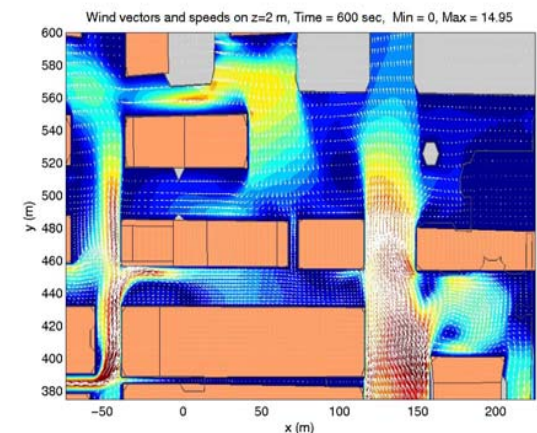
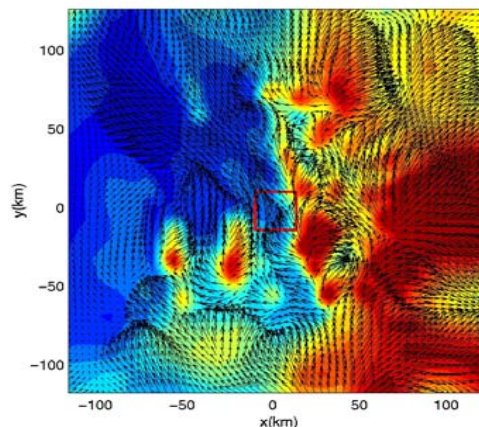
- DOE's center for emergency response to atmospheric releases of hazardous materials, the **National Atmospheric Release Advisory Center**, is located at LLNL
- NARAC's team of operational meteorologists, atmospheric scientists, and computer scientists calculate plume dispersion predictions for:
 - Emergency response
 - Vulnerability studies
 - Risk assessment
 - Intelligence applications





Research science and modeling efforts support NARAC

- Design, execution, and analysis of **field campaigns** for verification and validation of NARAC's meteorological and transport/dispersion models
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Oklahoma City's Joint Urban 2003 experiment: the largest urban dispersion experiment ever conducted



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Design Objectives:

- Document horizontal and vertical dispersion of SF₆ tracer in urban area
 - Fast (1 Hz) tracer measurements close to source
 - Tracer measurements up to 4 km from source
 - Continuous and instantaneous releases of tracer
- Document flow structure within and around Oklahoma City urban area under near- neutral atmospheric stability and moderate winds (>5 m/s)
 - Boundary layer height data
 - Surface energy budget data
 - Special focus on street canyon study
 - Traffic-induced turbulence study
- Document outdoor/indoor infiltration rates

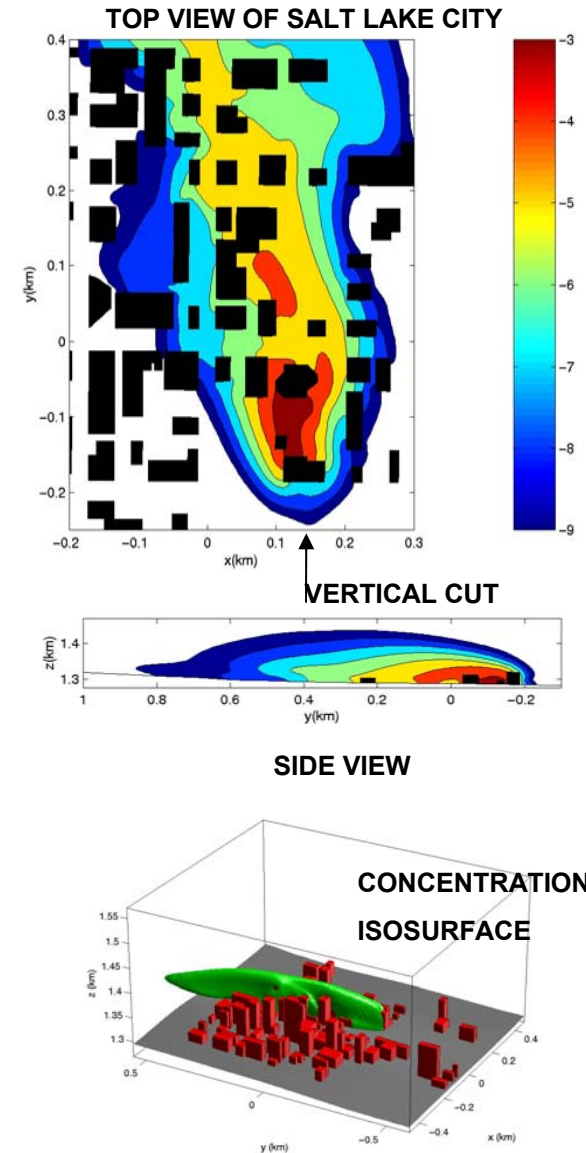
2 Terabytes of data!

- 150 Sonic Anemometers
- 20 Remote wind sensors
- 30 surface met stations
- 240 SF₆ sampling devices
- 7 level SF₆ on tower

Can our urban computational fluid dynamics model accurately simulate flow and transport in the urban center?



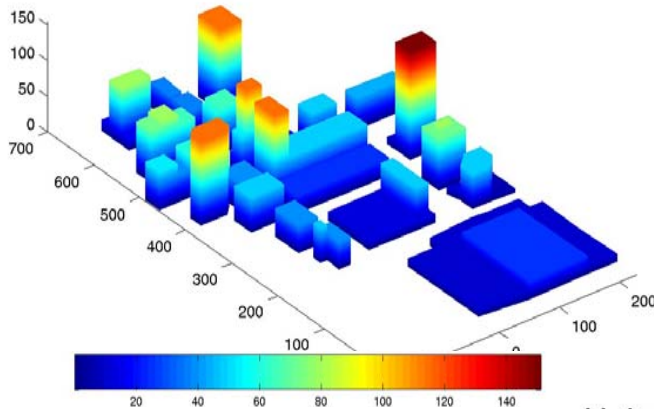
- High-fidelity, computationally-efficient dispersion simulations are essential for
 - Vulnerability studies and risk assessment
 - Critical infrastructure protection
 - Attribution and signature analysis
 - Intelligence applications
 - Emergency response
- NARAC's FEM3MP is
 - Massively parallelized CFD model based on solving 3-D time- dependent Navier-Stokes equations for large-scale problems
 - Finite elements
 - Multiple simple/advanced turbulence closures
 - Simple sub-models for canopies, aerosols, UV radiation decay, surface heating, etc.
 - Validated against data (wind tunnel, urban experiments)
- Innovative mixed explicit-virtual building representation decreases computational expense while still retaining accuracy in consequential areas



To save on computational cost, CFD simulations apply a mixed virtual-explicit building approach – is it reliable?

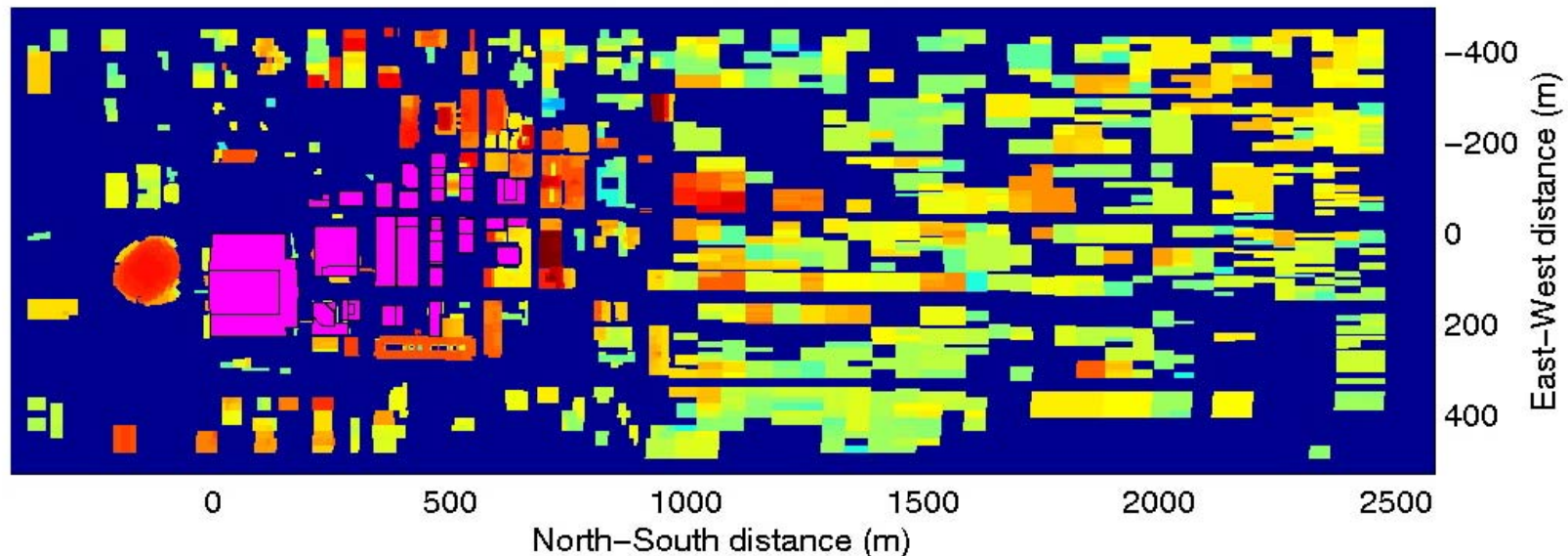


Explicitly resolved buildings



- Buildings in immediate proximity to source of tracer release are resolved explicitly
- Other buildings are represented as roughness elements

Total domain

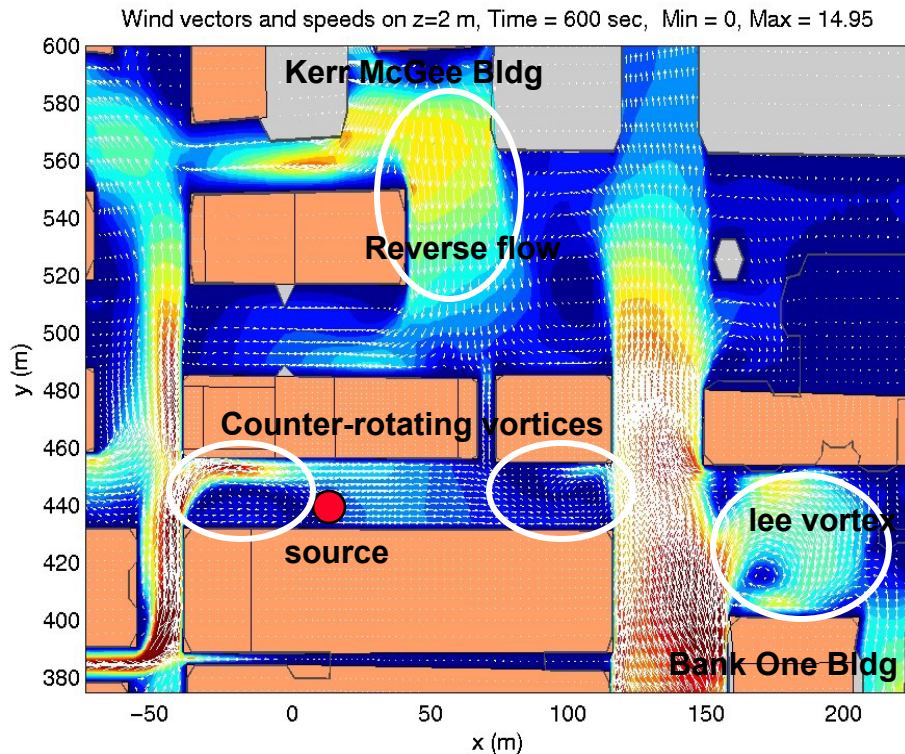


IOP 9: Simulated winds agree well with observations in OKC downtown area ($z = 8$ m)

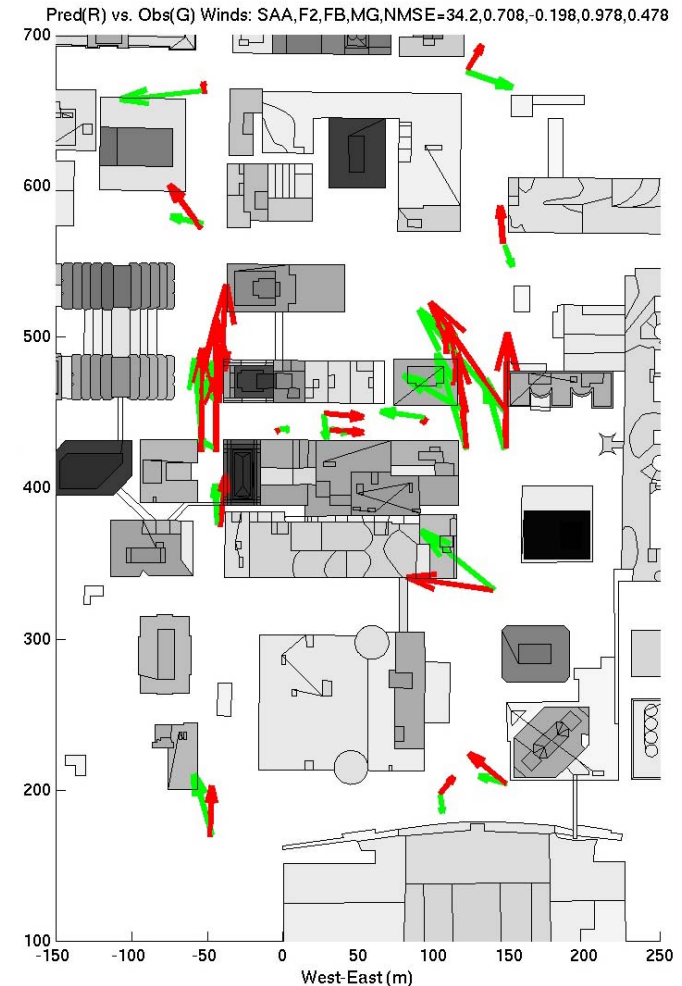


— Model
— DPG PWIDS Data

Predicted wind vectors in source area



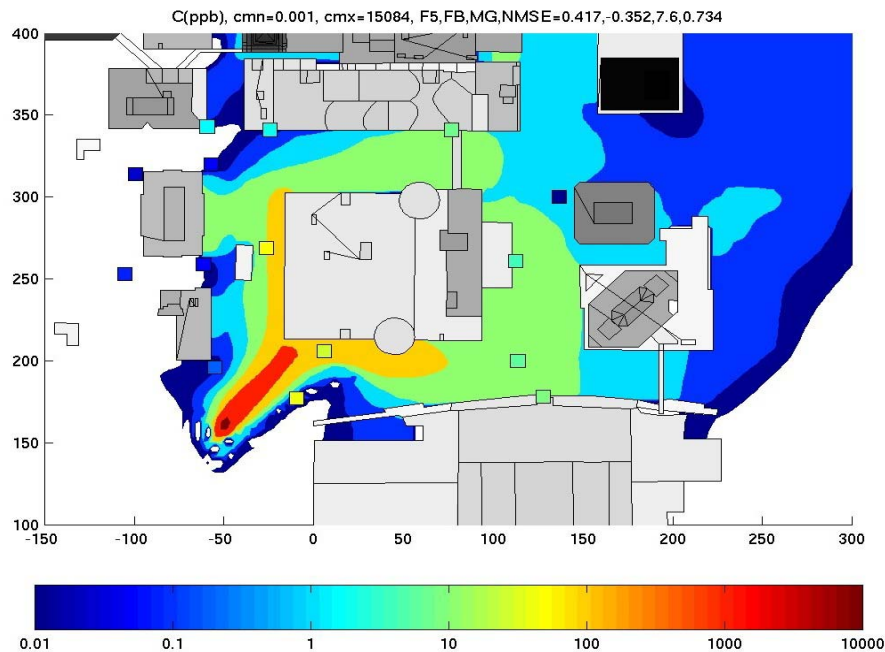
Predicted vs. observed wind vectors



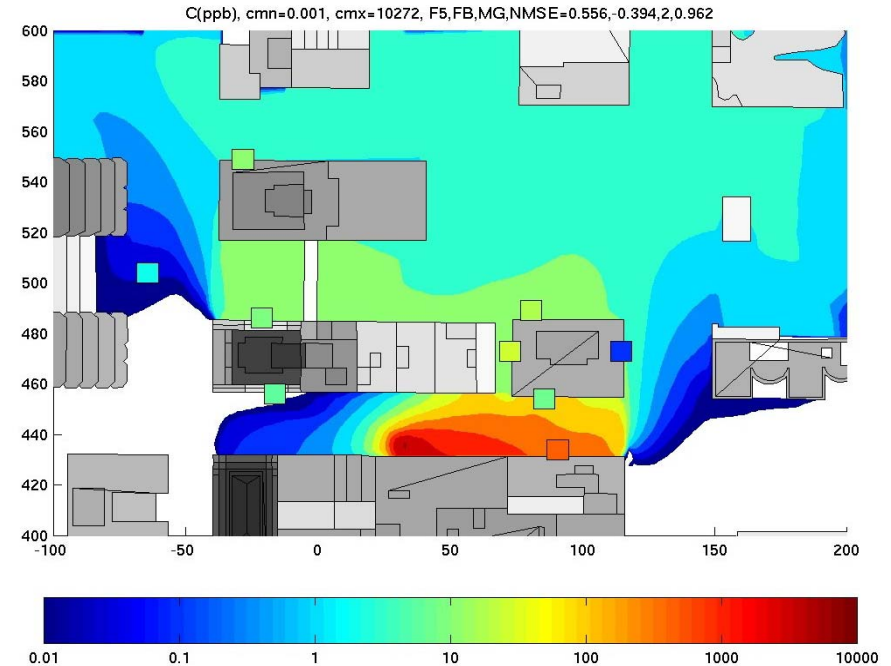
In the source region, predictions of concentrations agree well with observations



Predicted vs. observed concentration, IOP 3



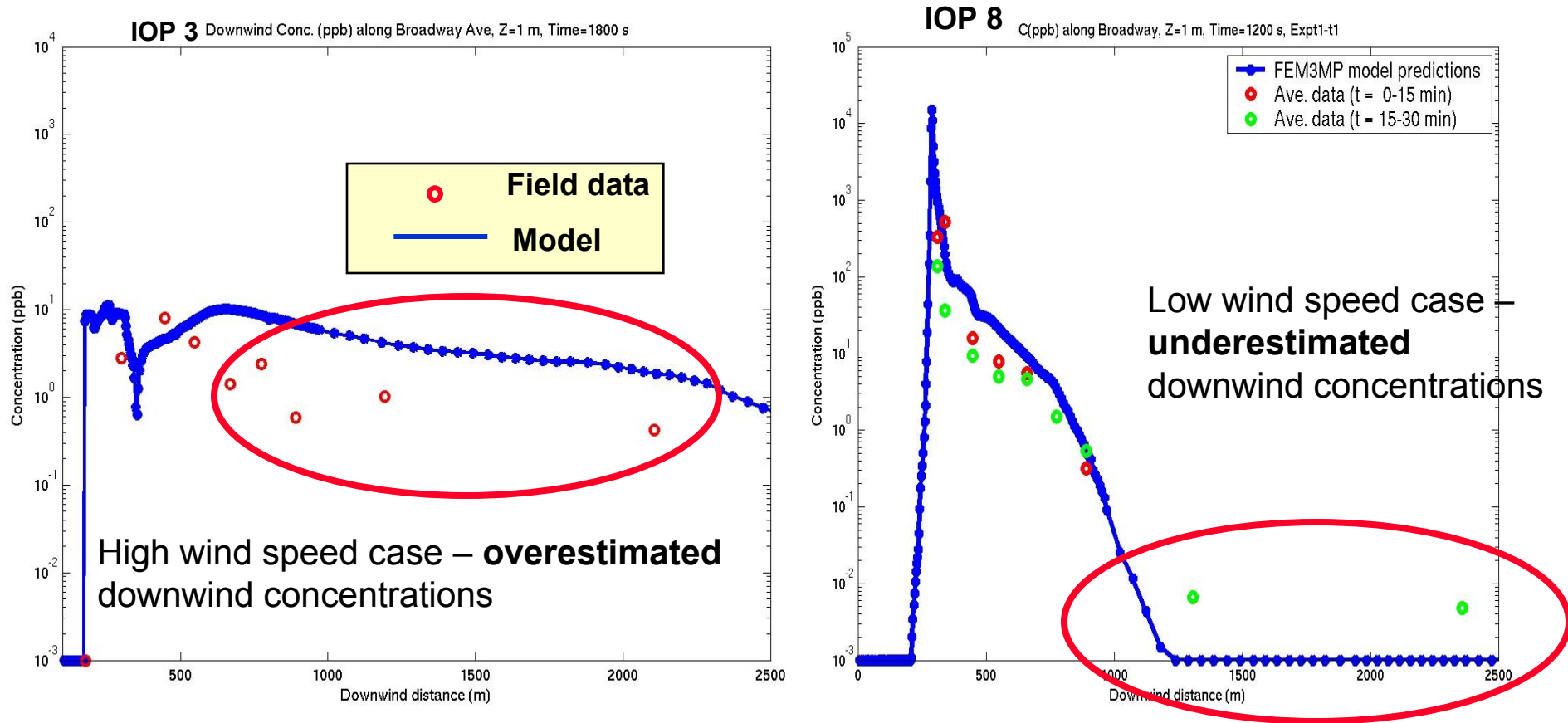
Predicted vs. observed concentrations, IOP9



Contours – model predictions
Small squares – observations

The agreement implies that in this region, the relevant turbulent mixing processes are accounted for and modeled properly.

Concentrations outside of the central business district indicate limits of the model's assumptions



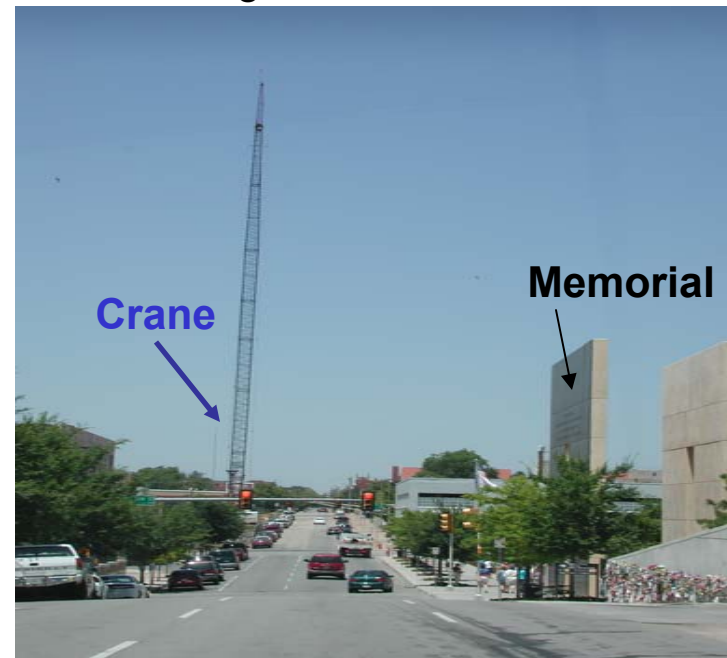
In high wind speed cases, we underestimate turbulent mixing, and in low wind speed cases, we overestimate turbulent mixing outside the CBD – other physical processes are at play.

LLNL's crane pseudo-tower provided vertical profiling of high-rate turbulence measurements downwind to help understand urban turbulence processes



- **Top of pseudo-tower anchored to crane; bottom anchored to a massive weight to maintain tension and minimize swaying or twisting**
- **Sonic anemometers (10 Hz R. M. Young model 81000) located at 8 levels, 8 – 83m**

Looking north from downtown



Looking east from westside



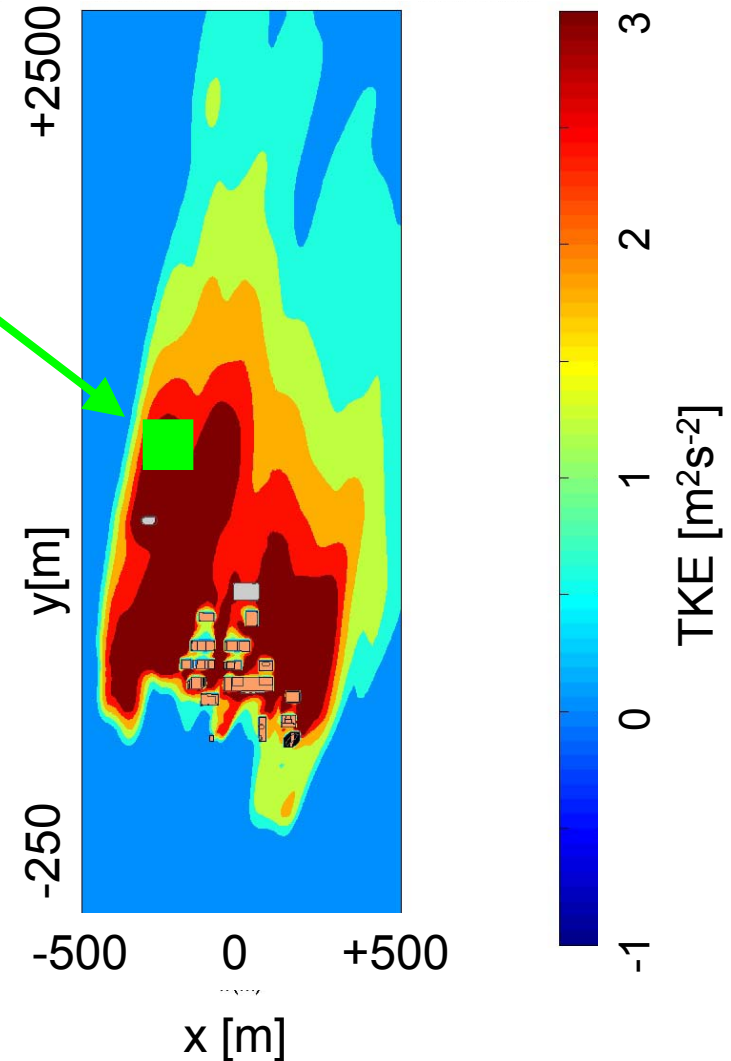
Located ~ 750m downwind of the central business district, the crane profile samples downwind of the urban core



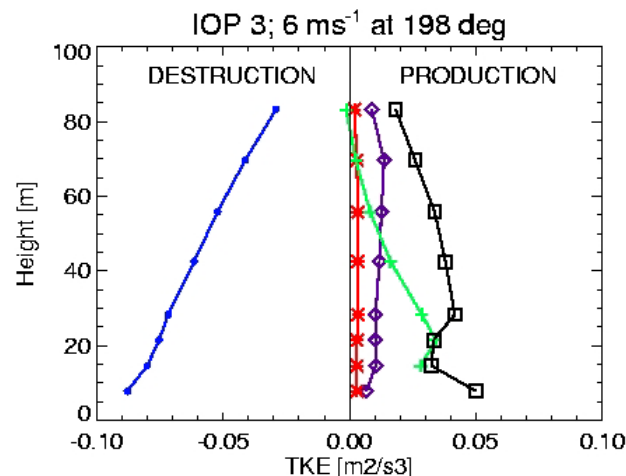
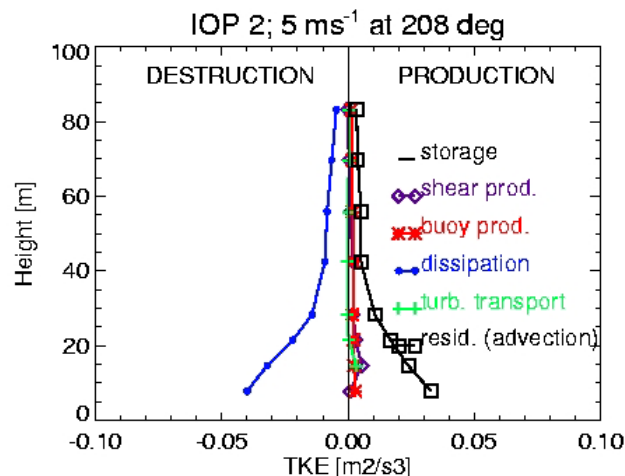
Crane is located at ~ (-200, 1200) m in a domain centered at the south edge of downtown (intersection of Broadway and Sheridan).

Eight levels of sonic anemometers provide 10Hz measurements of wind speed and virtual temperature, allowing estimates of fluxes and turbulent kinetic energy.

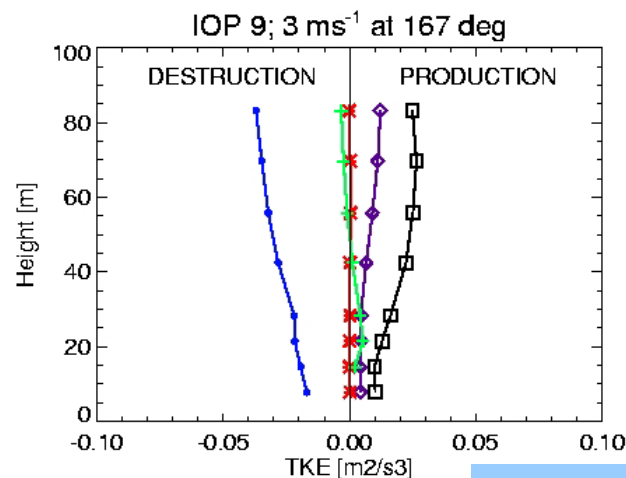
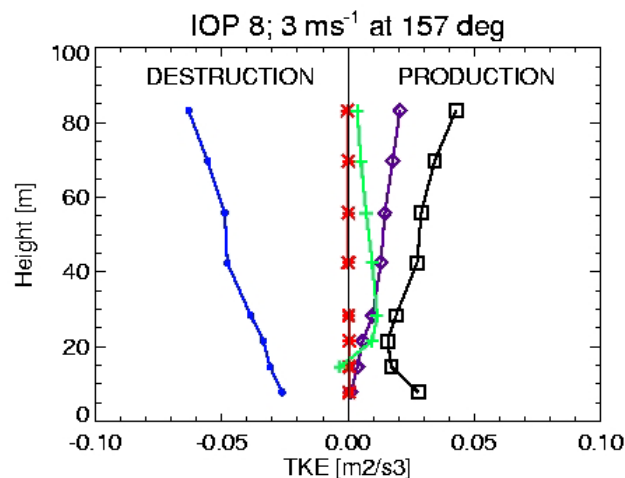
These contours of TKE at a height of 50 m illustrate the increased production of TKE in the city center, as well as the wake induced by buildings too short to appear in this slice.



Our analysis of turbulent budgets show that advection of turbulence is a major component of urban wind profiles that must be parameterized appropriately for accurate simulations



Daytime IOPs show TKE production and destruction decreasing with height

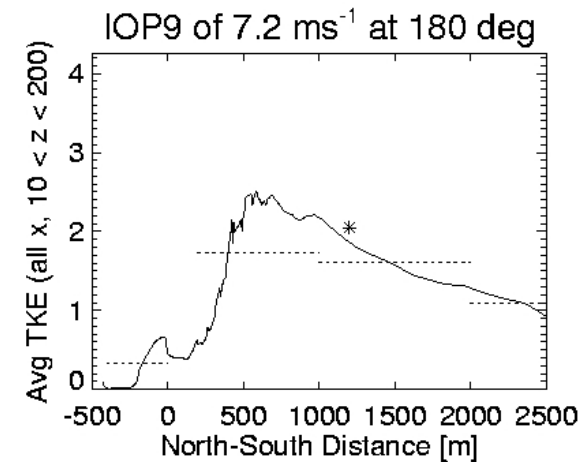
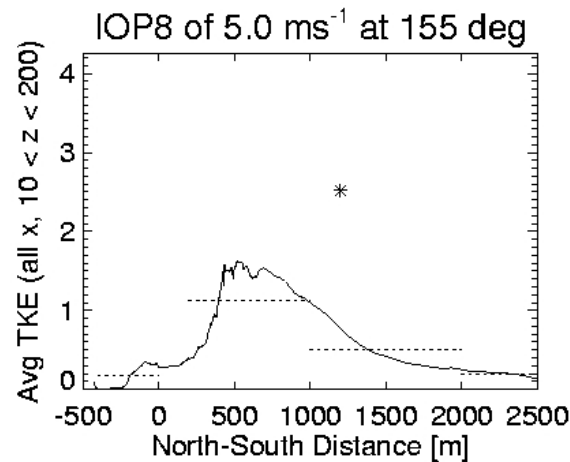
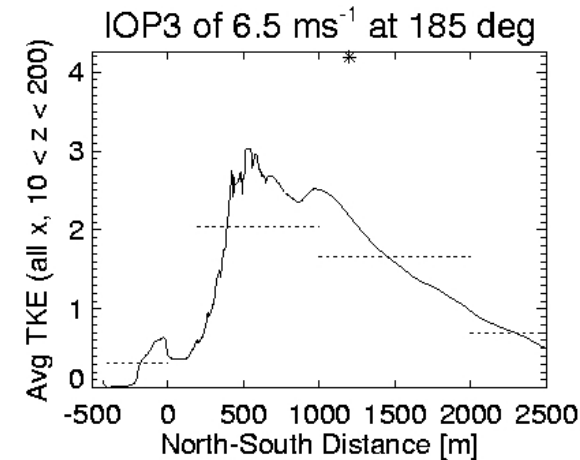
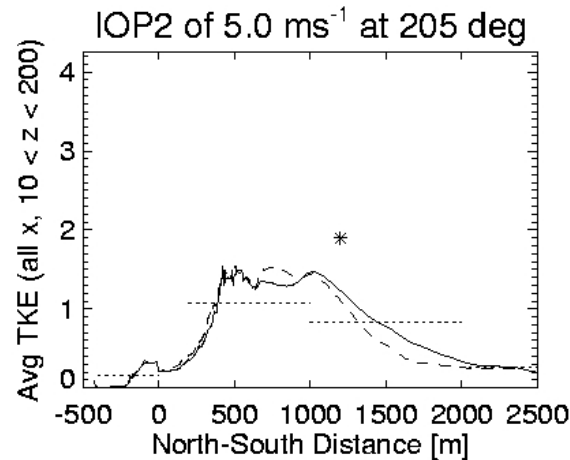
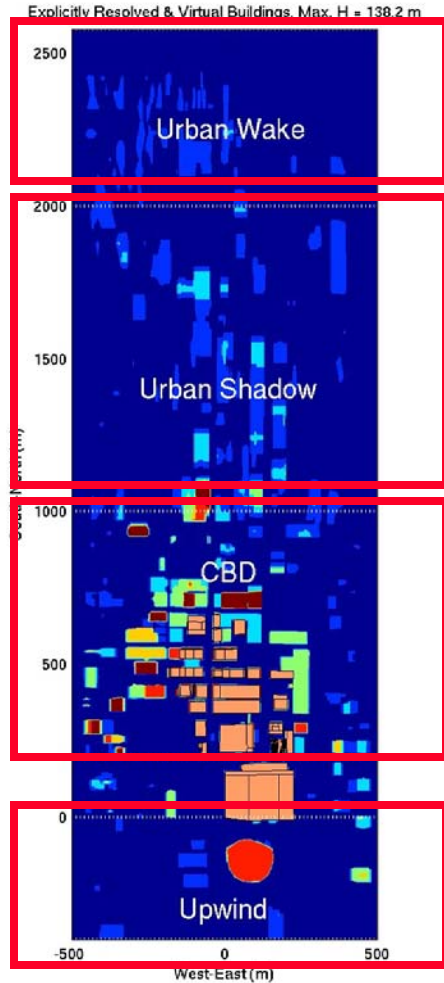


Nighttime IOPs show TKE production and destruction increasing with height

From Lundquist & Chan, *JAMC*, 2007

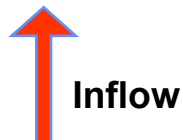
In every case analyzed, the advection term dominates the TKE budget. Most current turbulence models do not properly account for advection and its effects.

Urban-generated turbulence decays downwind; penetrates further in higher wind speed cases



From Lundquist & Chan, *JAMC*, 2007

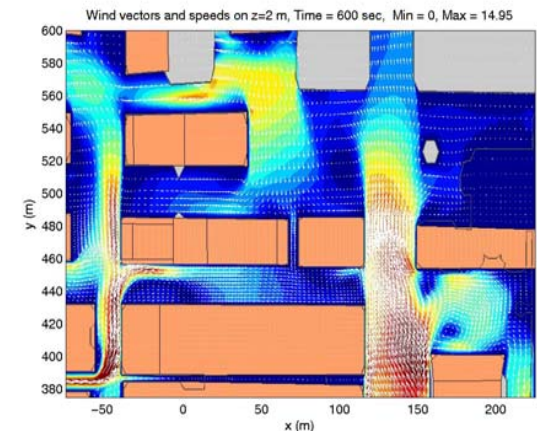
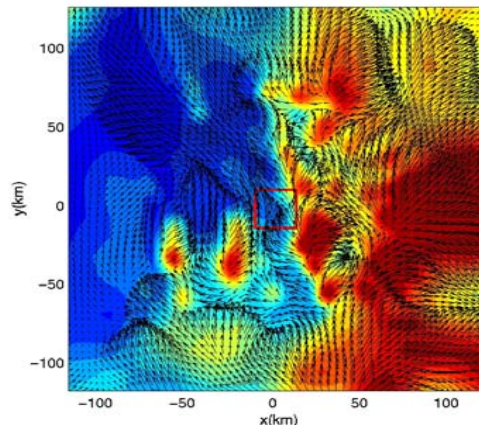
In urban shadow & urban wake zones, other means of TKE production regain primary influence – increased role of mesoscale phenomena like LLJs





Research science and modeling efforts support NARAC

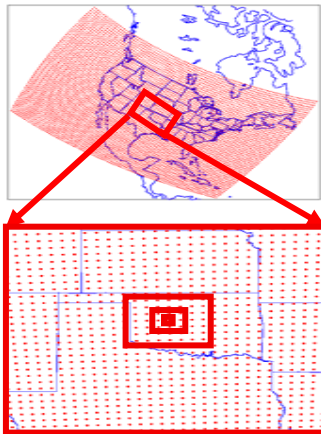
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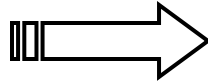
Motivated by these results, we are improving an NWP model to do a better job in urban areas and complex terrain



Numerical weather prediction (NWP) models capture large scale motions and changing weather ($\Delta x \sim 12$ km)

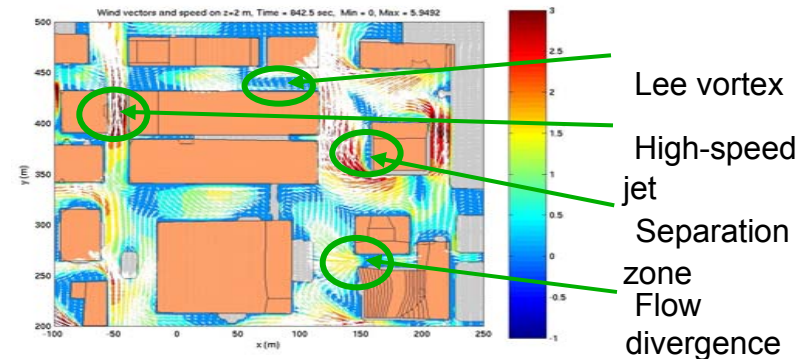


How to fill this gap?



...but at higher resolution, 1) NWP parameterizations are inappropriate and inaccurate, and 2) coordinate systems cannot capture complex terrain of urban environment

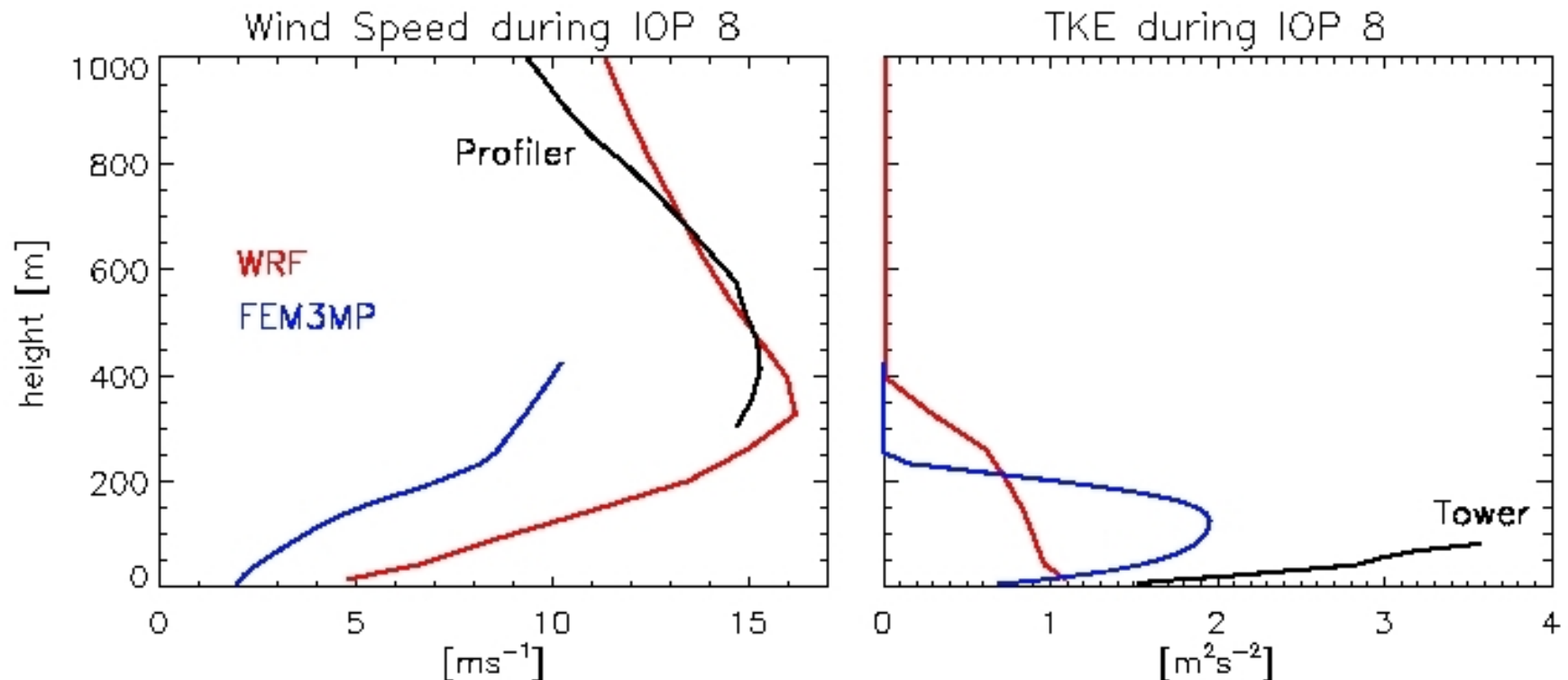
Computational Fluid Dynamics (CFD) urban models capture intricacies of building-induced turbulence ($\Delta x \sim 5$ m)



...but CFD models have difficulty incorporating changing and complex boundary conditions when the weather is variable

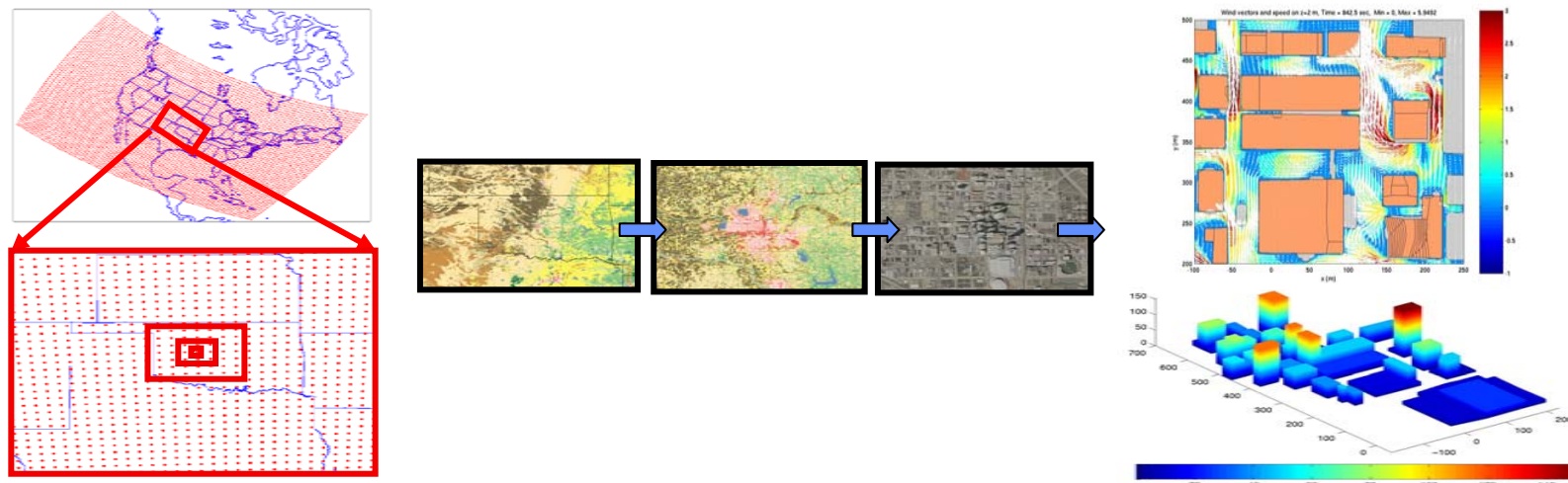


This gap is consequential! (Lundquist and Mirocha, 2007, JAMC)



- **WRF** is the new community-based numerical weather prediction model
- **FEM3MP** and **original WRF** simulated an IOP from Joint URBAN 2003
- IOP8 presents a complex mesoscale situation. **Original WRF** can capture the mean wind; neither **FEM3MP** and **original WRF** can capture turbulent mixing and diffusion processes
- Accurate simulation of wind and turbulent mixing in urban areas requires accuracy in
 - Large-scale weather prediction
 - High-resolution turbulence parameterizations
 - Representation of complex urban terrain and its effects

Our LDRD-funded effort will provide a powerful tool for studying atmospheric dispersion at multiple scales



Simultaneous integration of successively nested grids will resolve the entire spectrum of physical processes important for atmospheric dispersion in urban environments.



Atmospheric modeling system from NCAR

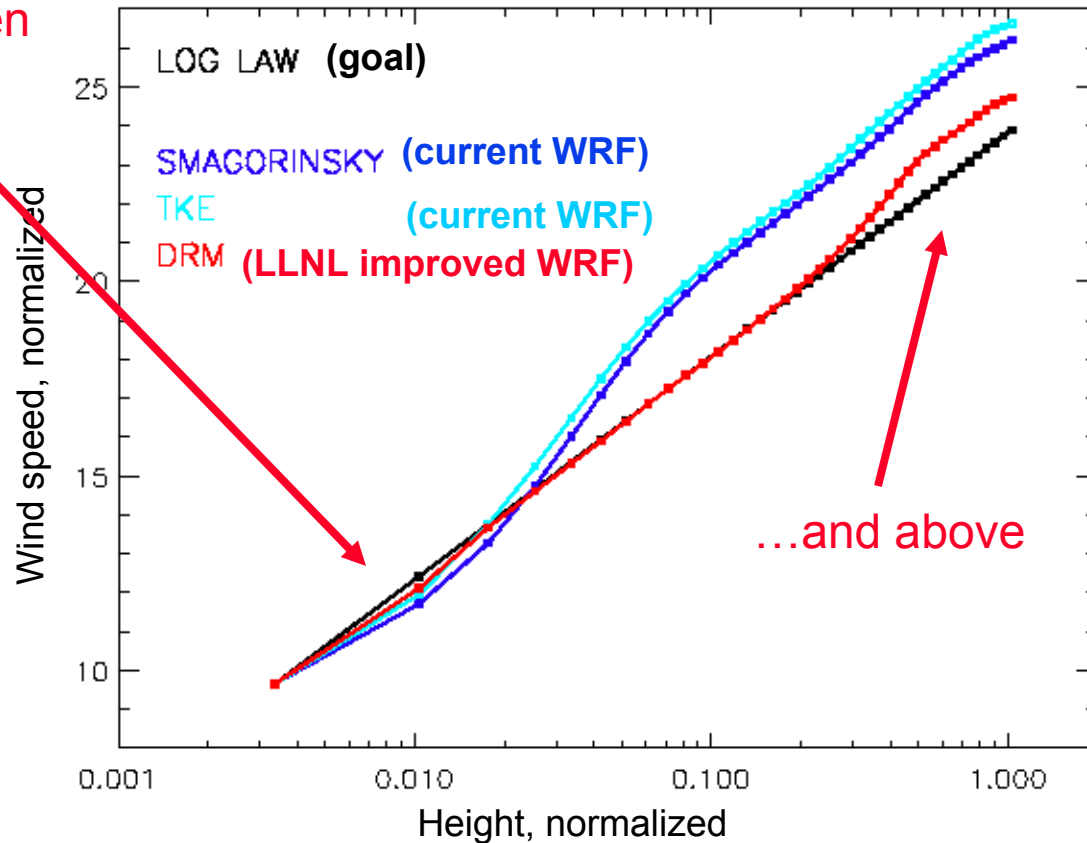
state-of-the-art numerics, multiple physics options, multiple 2-way nesting, community development

Our team is extending WRF's capability to address urban scales by developing and implementing 1) improved turbulence modeling (DRM) and 2) complex terrain ability (IBM) to support LLNL's programs and to share with the larger community.

LLNL's "DRM" WRF improves accuracy of wind profiles compared to analytic solutions



Improvement seen
both near
the surface...

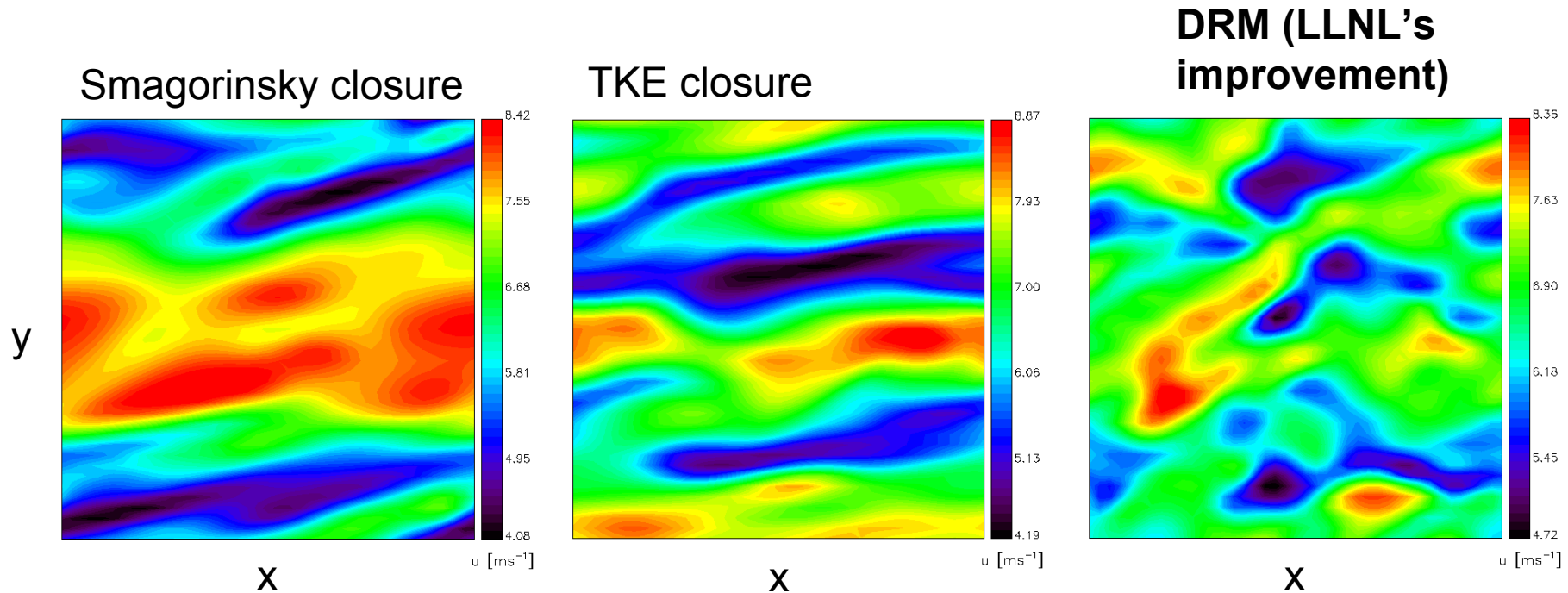


Results courtesy J. Mirocha, LLNL

LLNL's improved WRF simulates atmospheric flow more realistically than do existing WRF parameterizations



Plan view contours of instantaneous velocity using three turbulence parameterizations

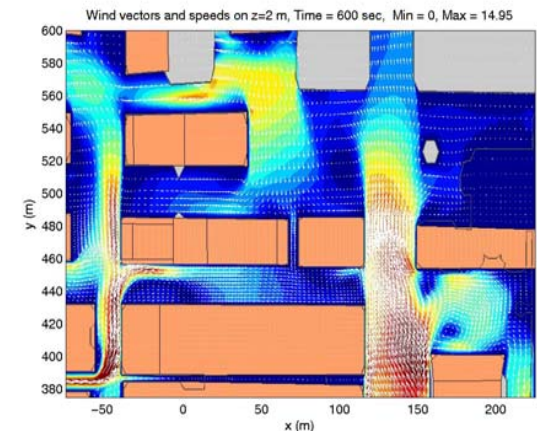
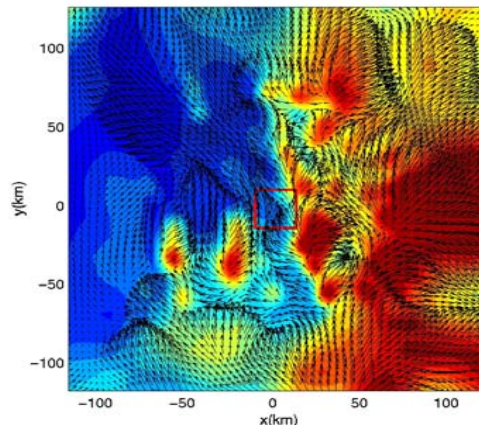


The “streaky” nature of WRF’s native parameterizations (left, center) are unrealistic. LLNL’s implementation of the DRM model (right) exhibits more realistic inhomogeneities.



Research science and modeling efforts support NARAC

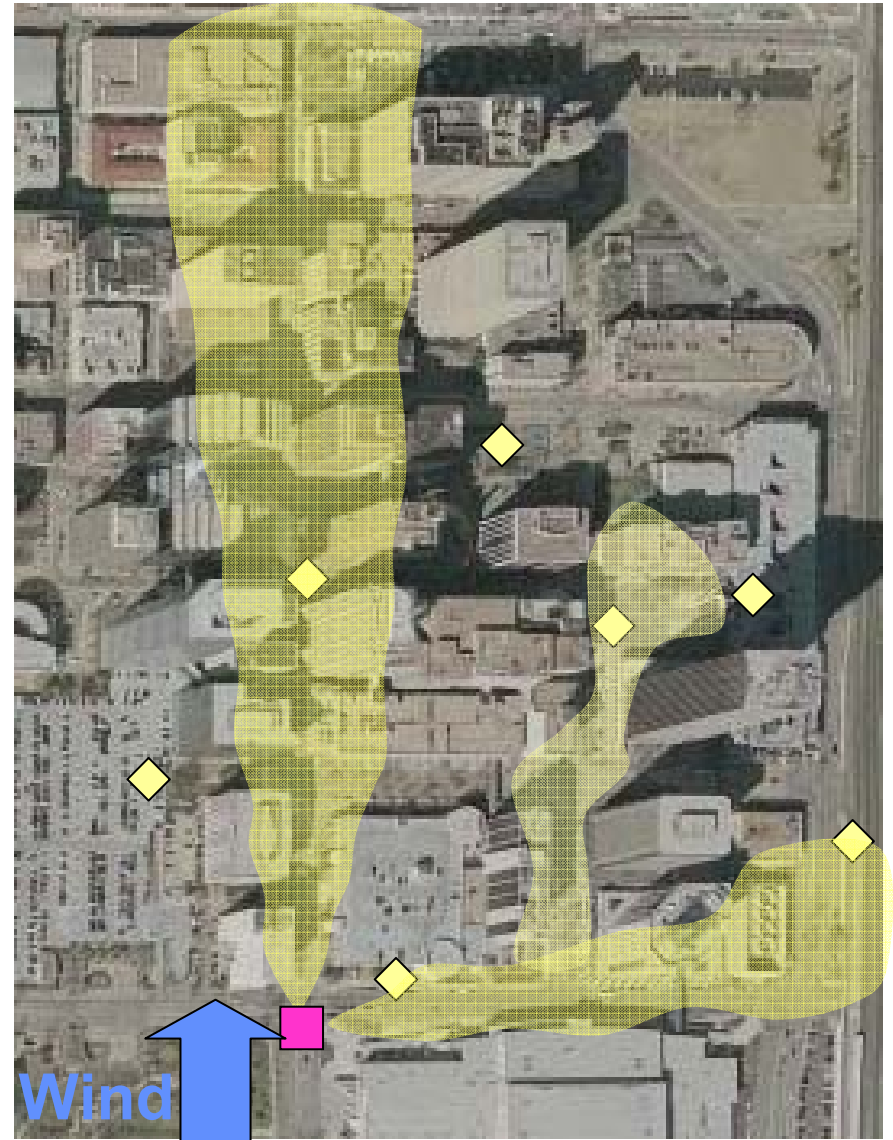
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Sparse measurements are often the only data available to describe an unknown atmospheric release.



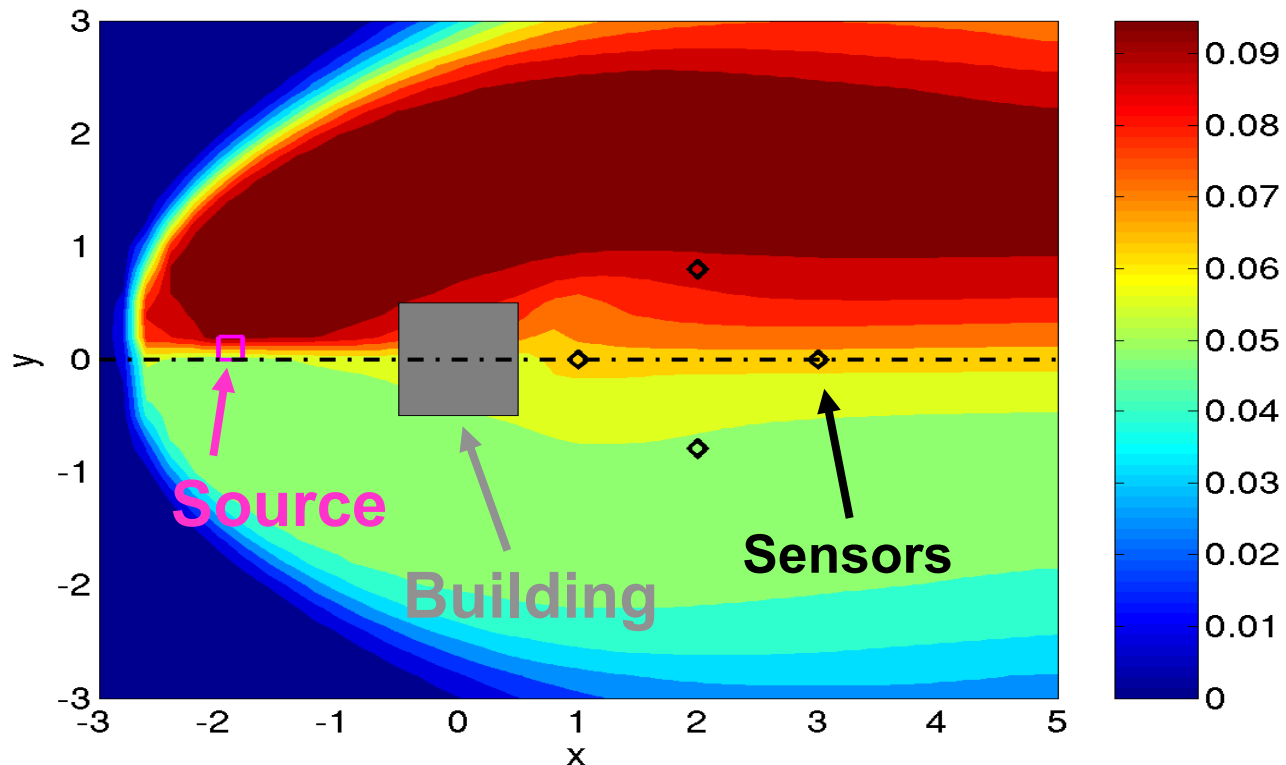
- Given a highly complex domain, with buildings of various shapes and sizes, and concentration measurements at a few locations, is it possible to find the source of a contaminant plume?



Prototype example consists of steady-state flow around a cube

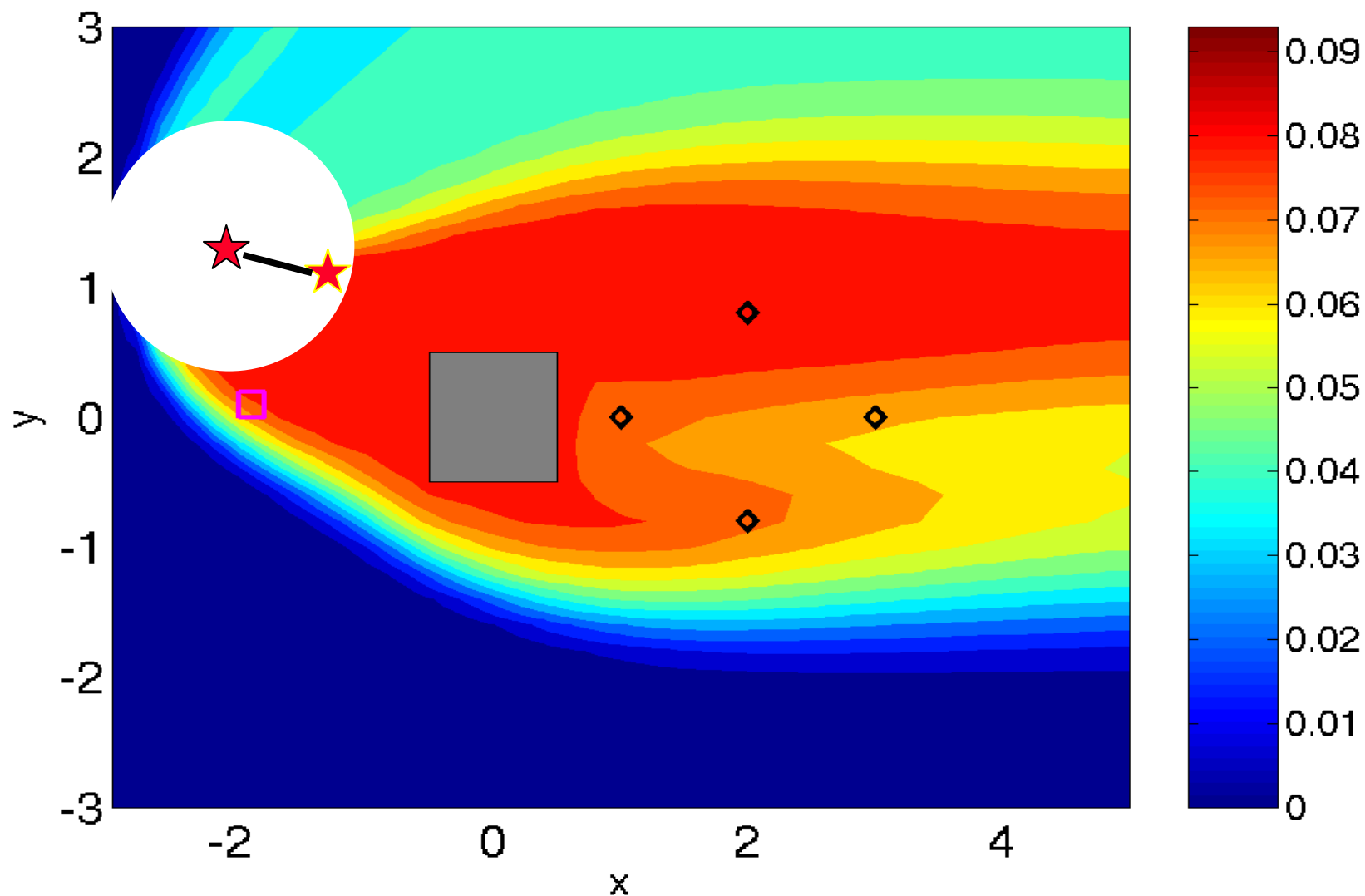


- Meteorology and dispersion calculated with 3D building-resolving FEM3MP Reynolds Averaged Navier-Stokes code
- Presence of building causes asymmetric plume
- Bayesian inference with stochastic sampling used to reconstruct source location and strength



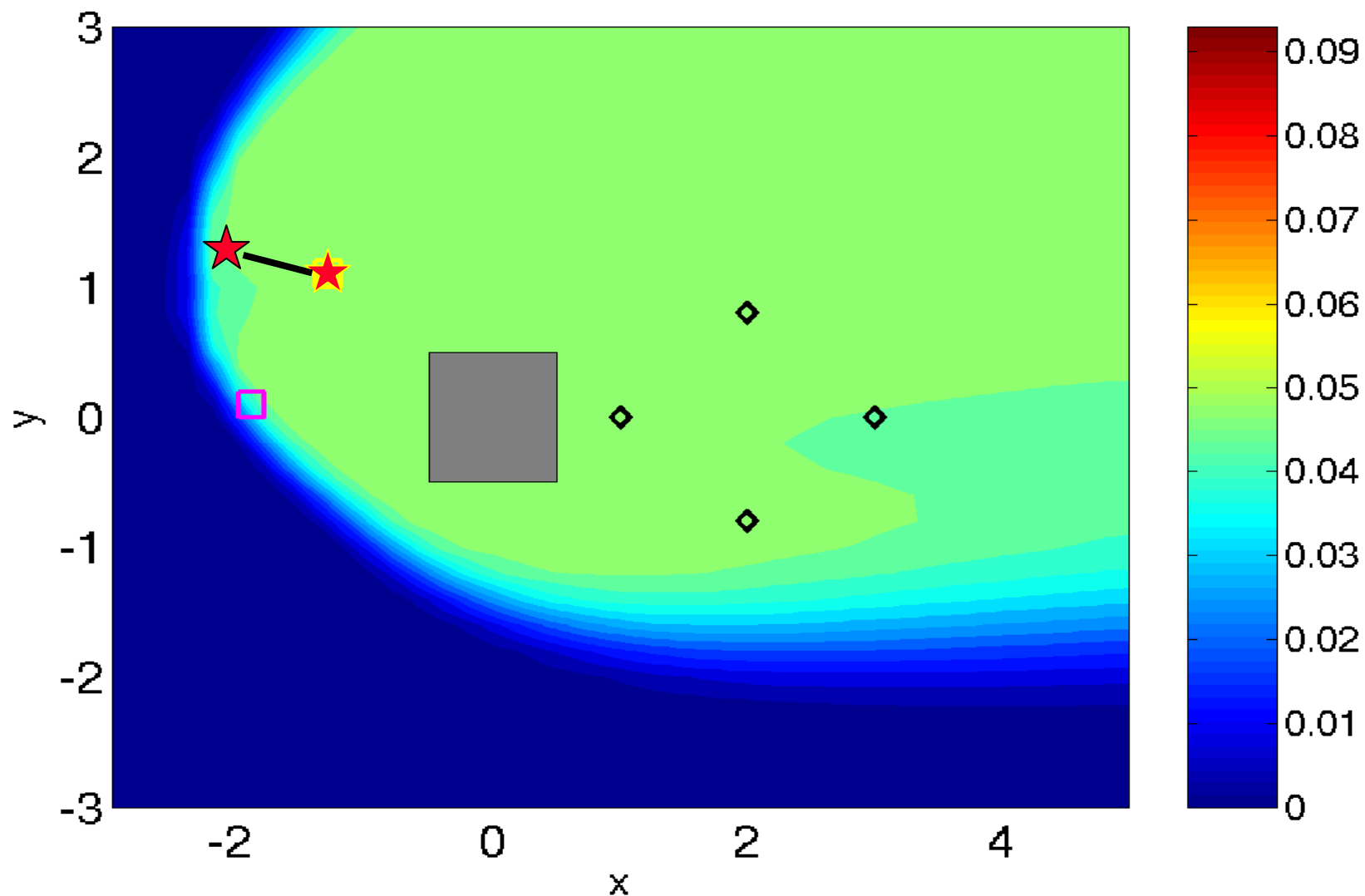
Markov Chain Monte Carlo for source inversion

- initial guess and new proposal



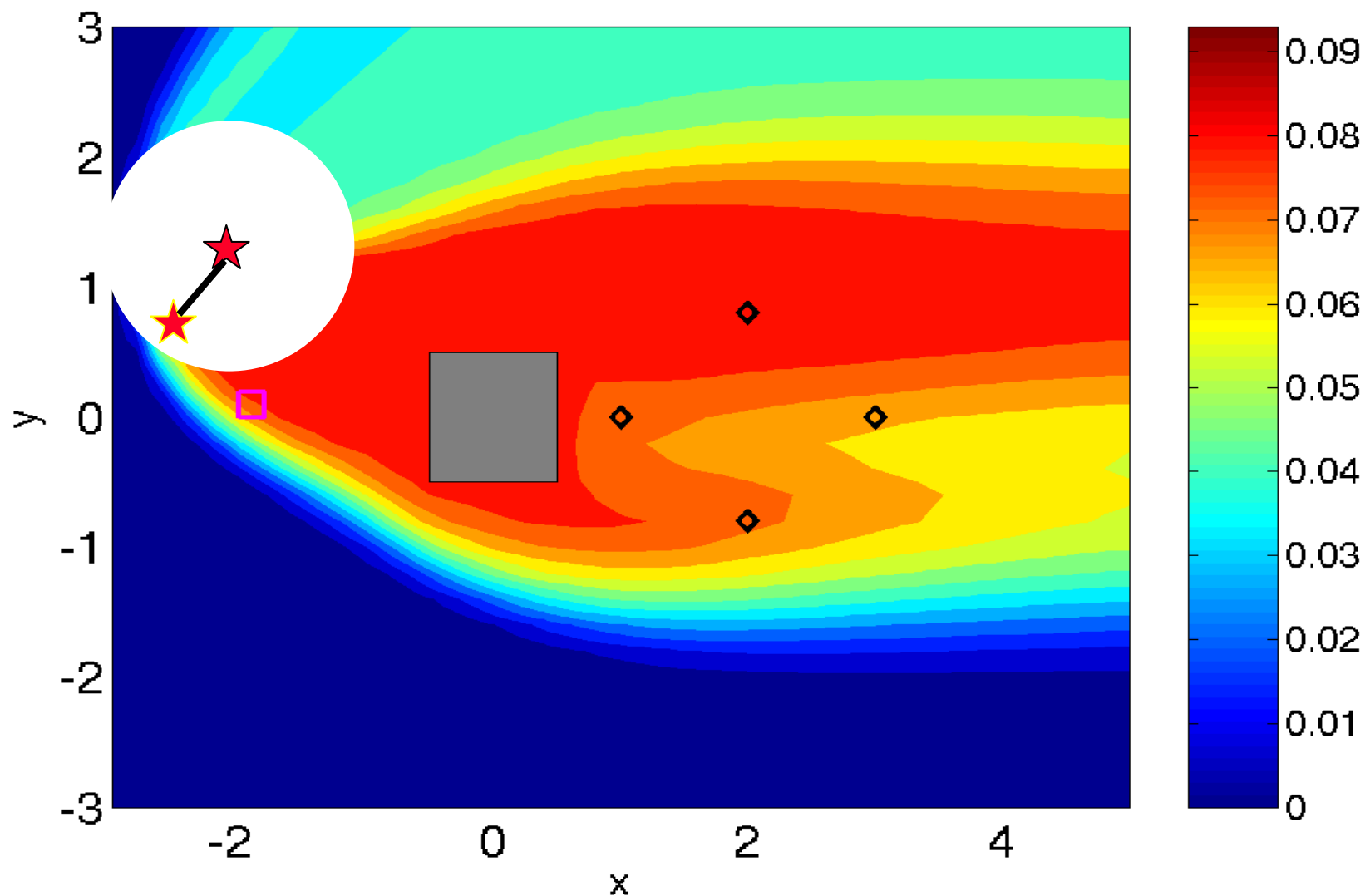
Markov Chain Monte Carlo for source inversion

- first proposal - rejected



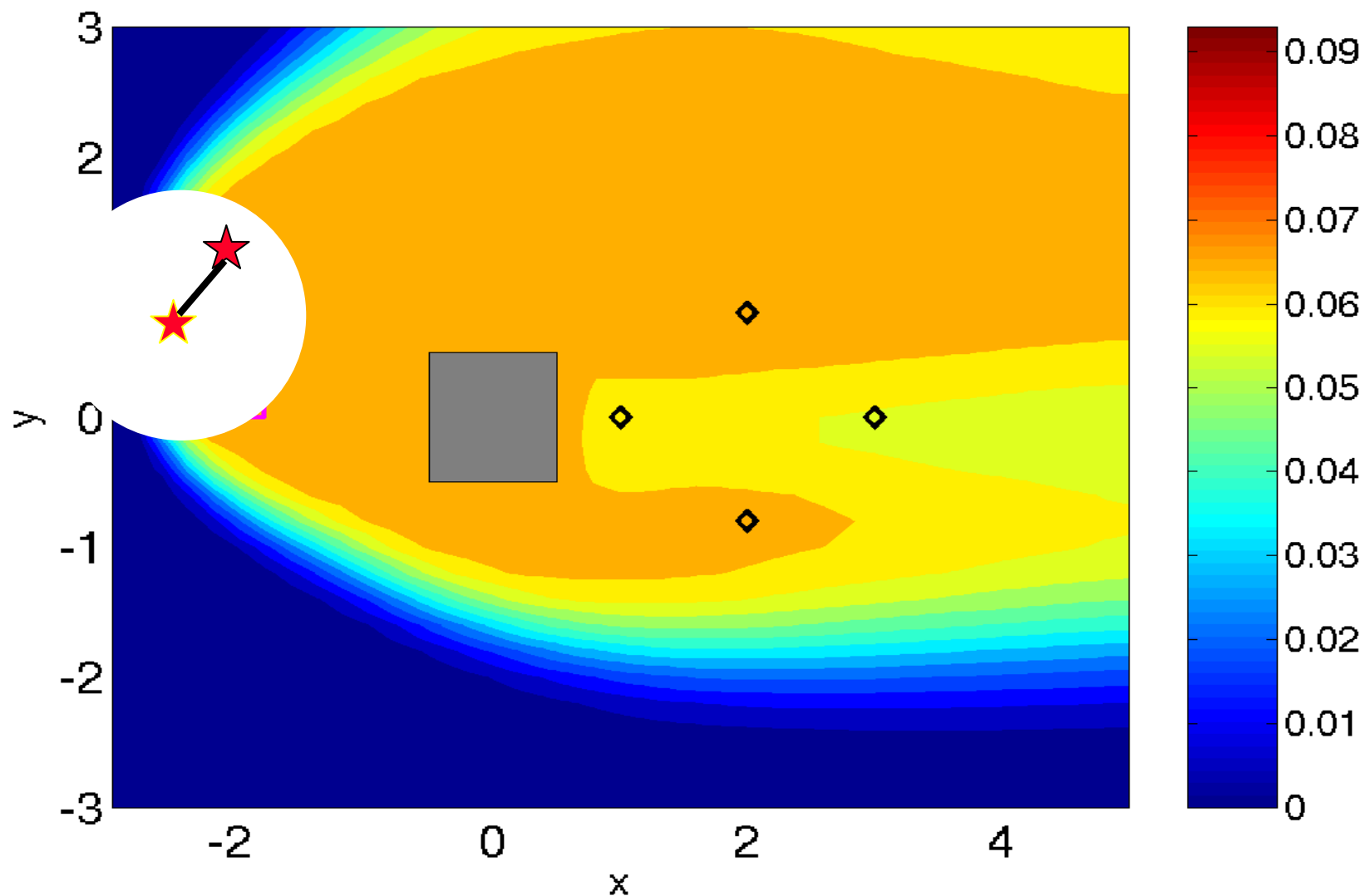
Markov Chain Monte Carlo for source inversion

- new proposal

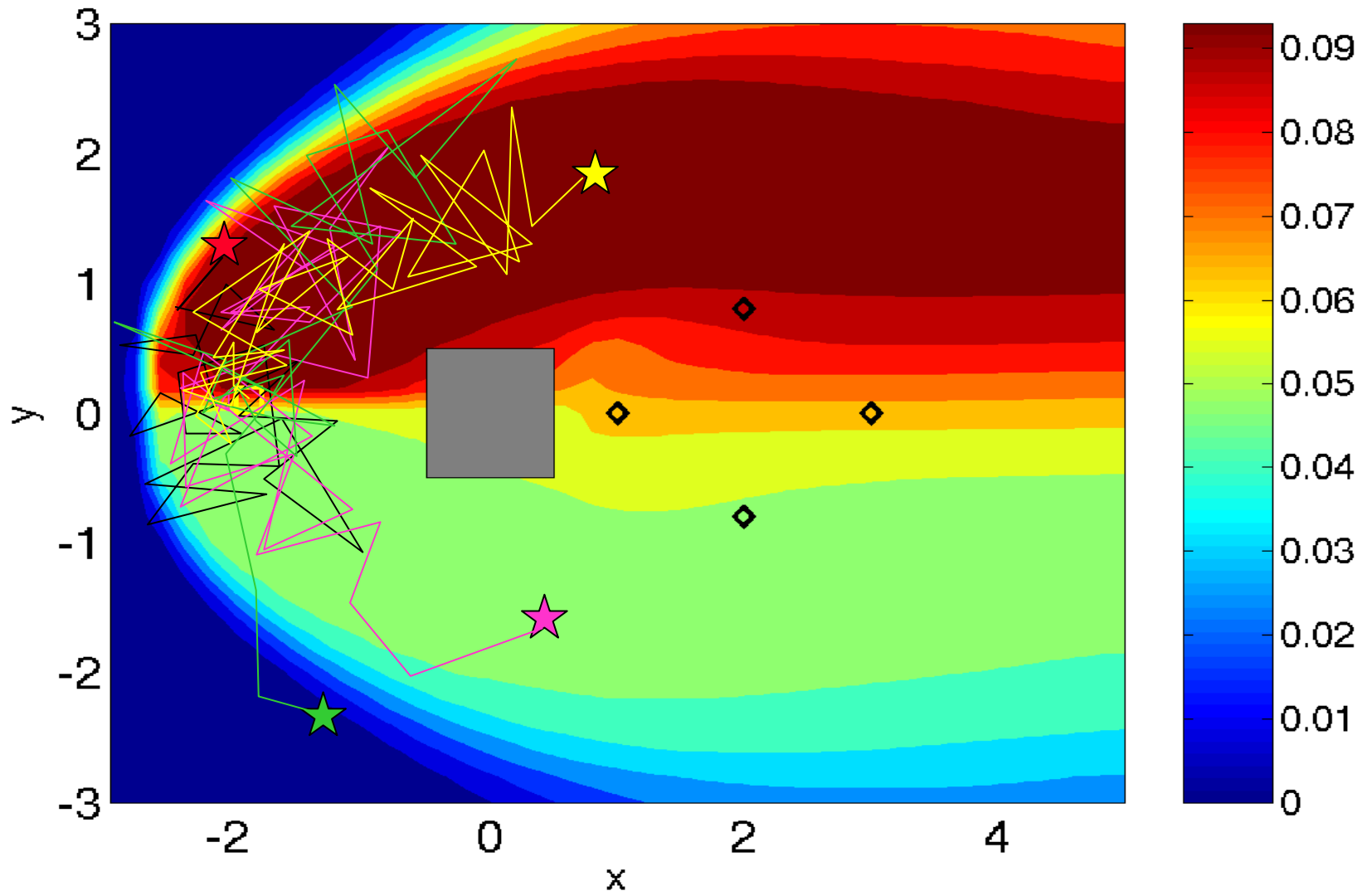


Markov Chain Monte Carlo for source inversion

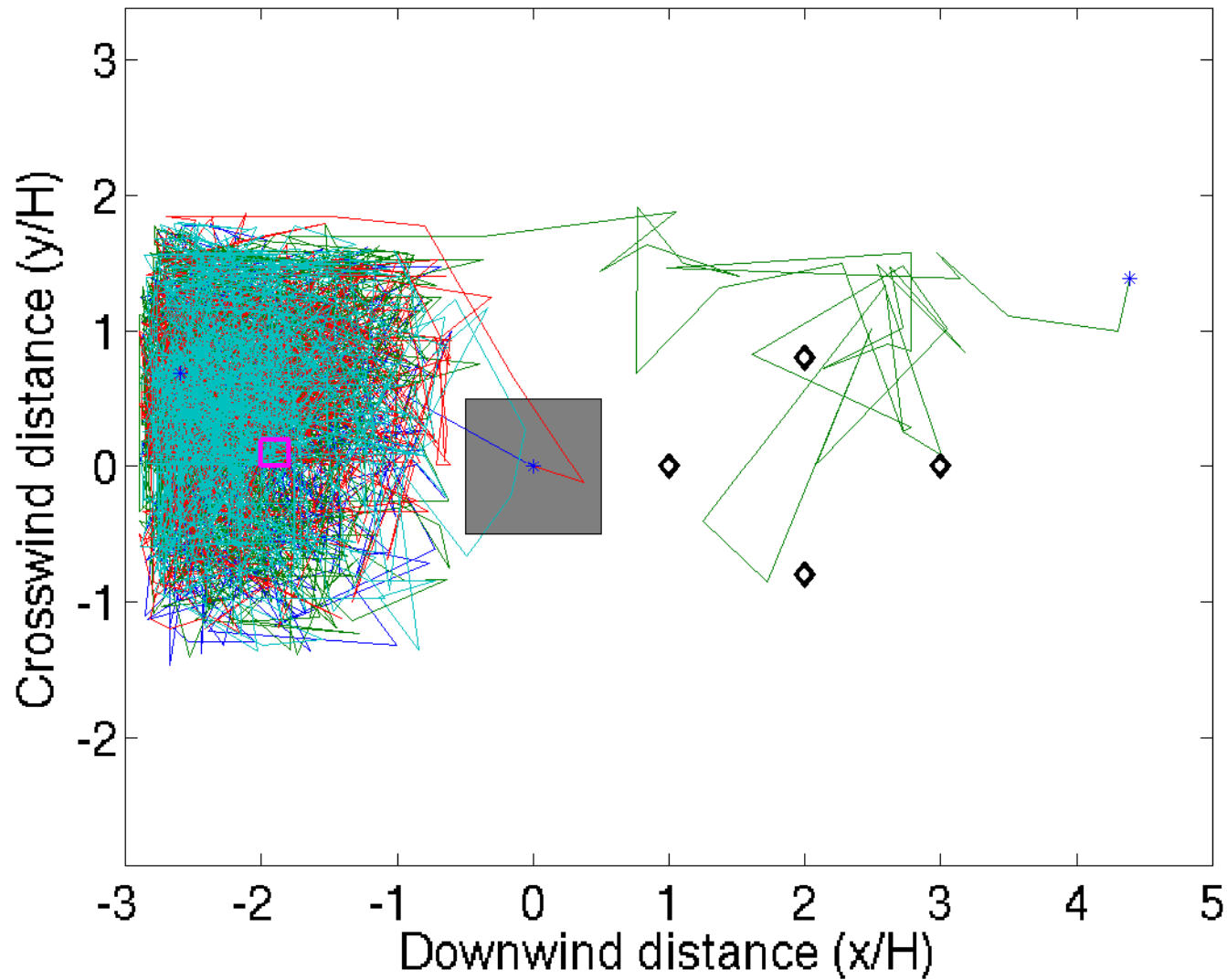
- new proposal - accepted



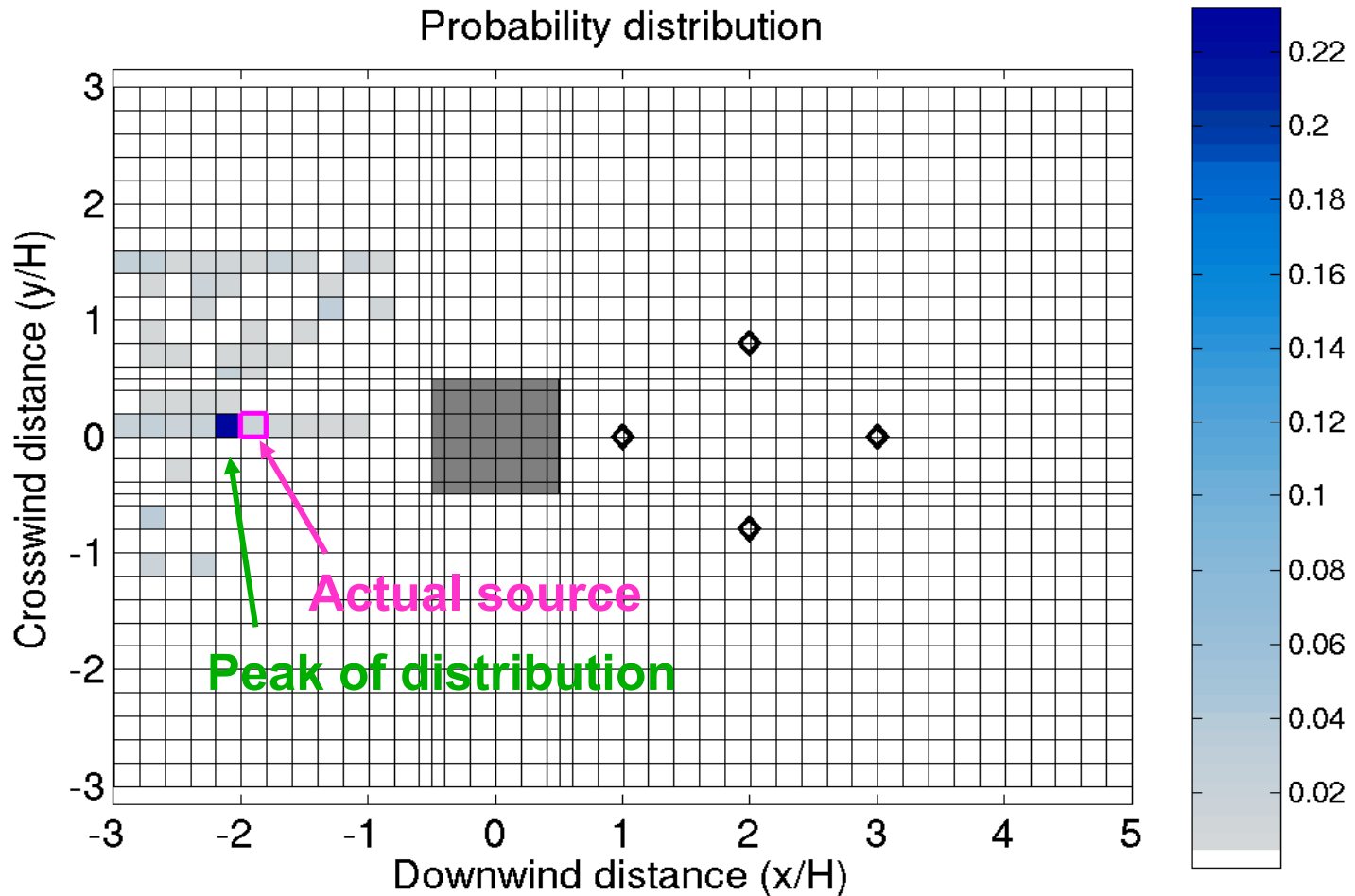
Multiple Markov chains, moving independently, converge on source



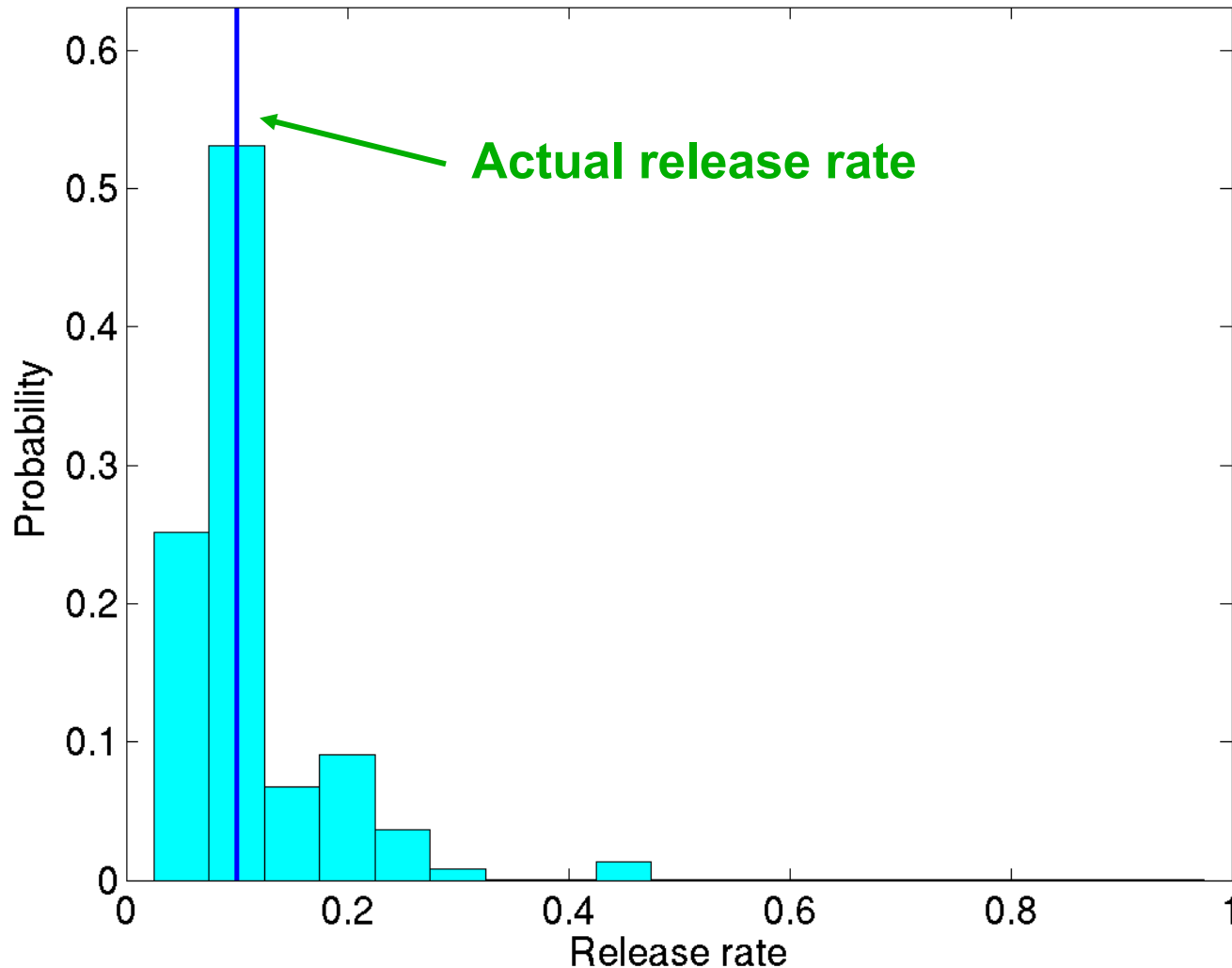
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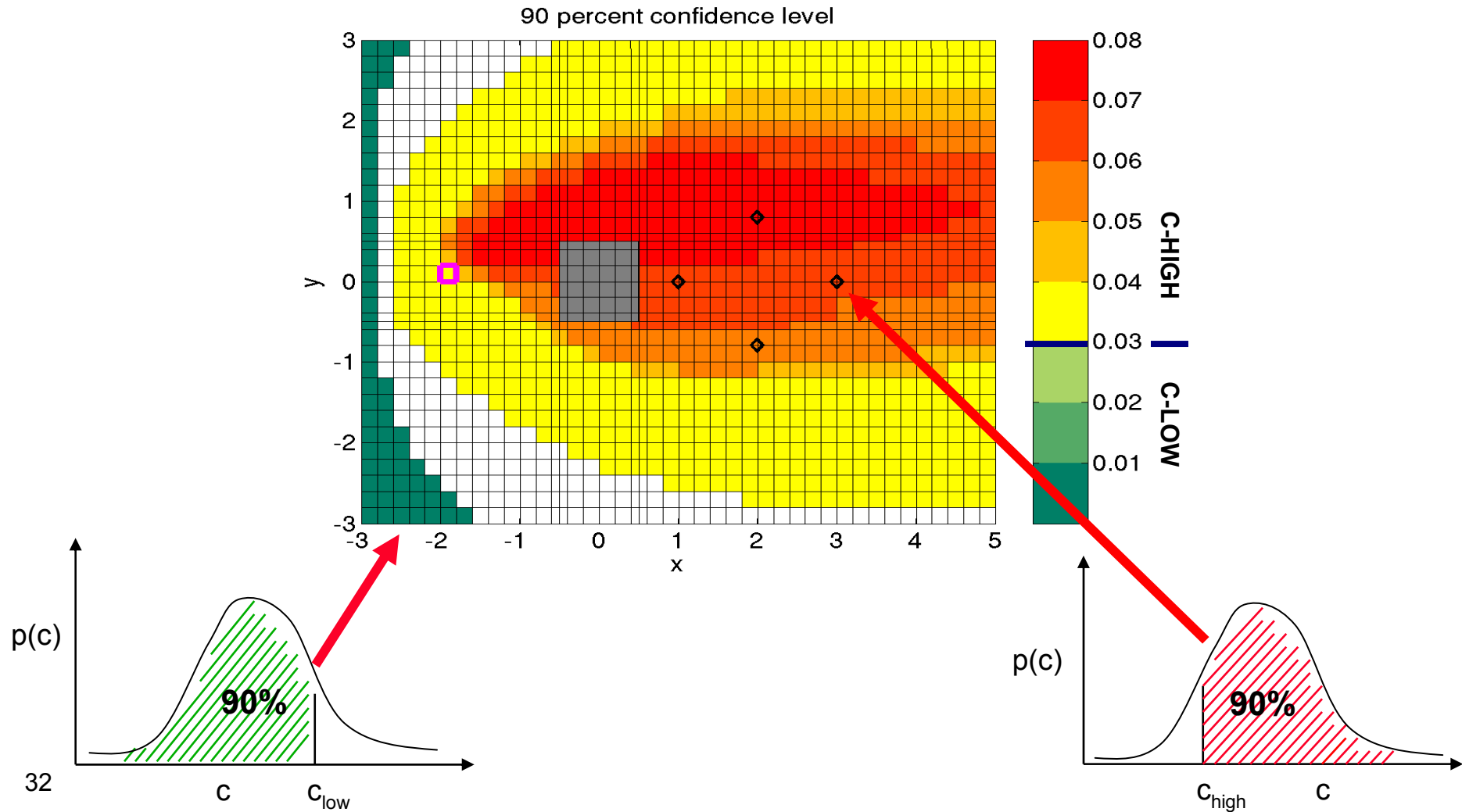
Information from all chains can be synthesized into a probability distribution of source location, defining most likely locations



Information from all chains can be synthesized into a probability distribution of release rate, indicating likely magnitude of release



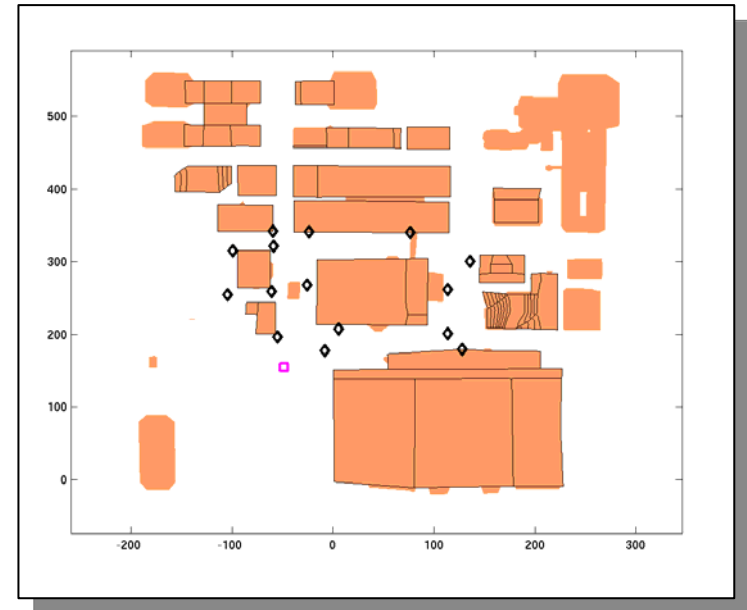
Information can be further aggregated into a composite plume, showing the most likely effects of the unknown release





Source inversion for Oklahoma City

- FEM3MP – 3D building-resolving forward model
- Joint URBAN 2003 daytime SF_6 release
- 133 x 146 x 30 grid size
- Approx 600 x 650 x 250 m domain
- Steady log profile inflow, southerly winds at $u_{z=50\text{m}} = 6.5 \text{ m/s}$
- Winds steady after ~10 min, used to drive dispersion simulations

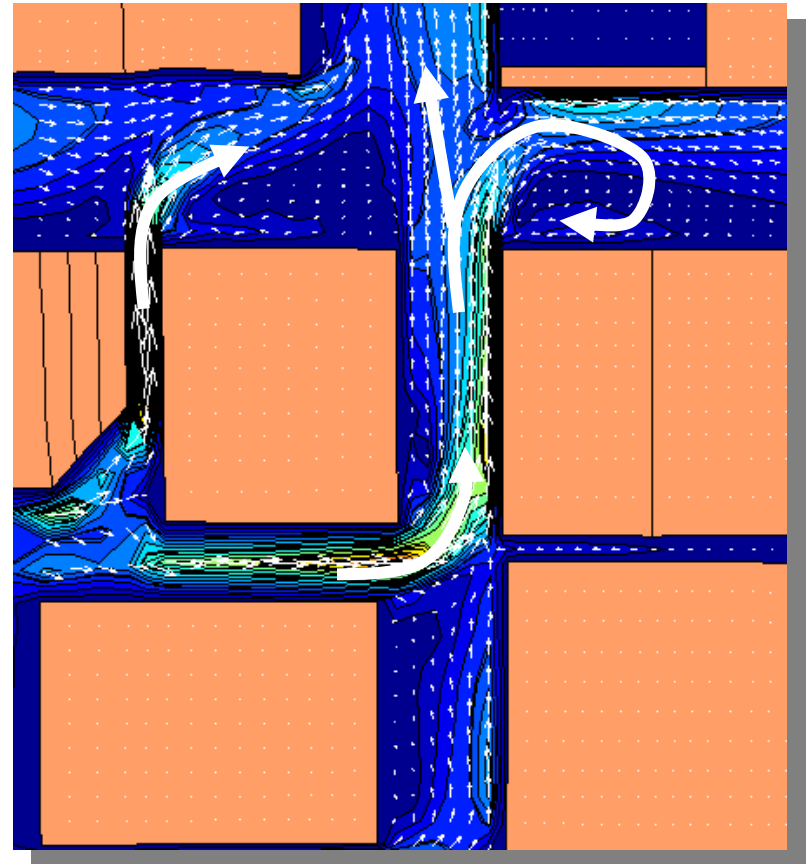


Chow et al., 2007, *JAMC*

Inversion must accommodate the complex meteorological flow which affected the release



- Plume splitting, corner eddies
- Max building height 120m
- Sheltering, updrafts
- Model error and assumptions are also considered.



Velocity vectors and horizontal wind speed contours

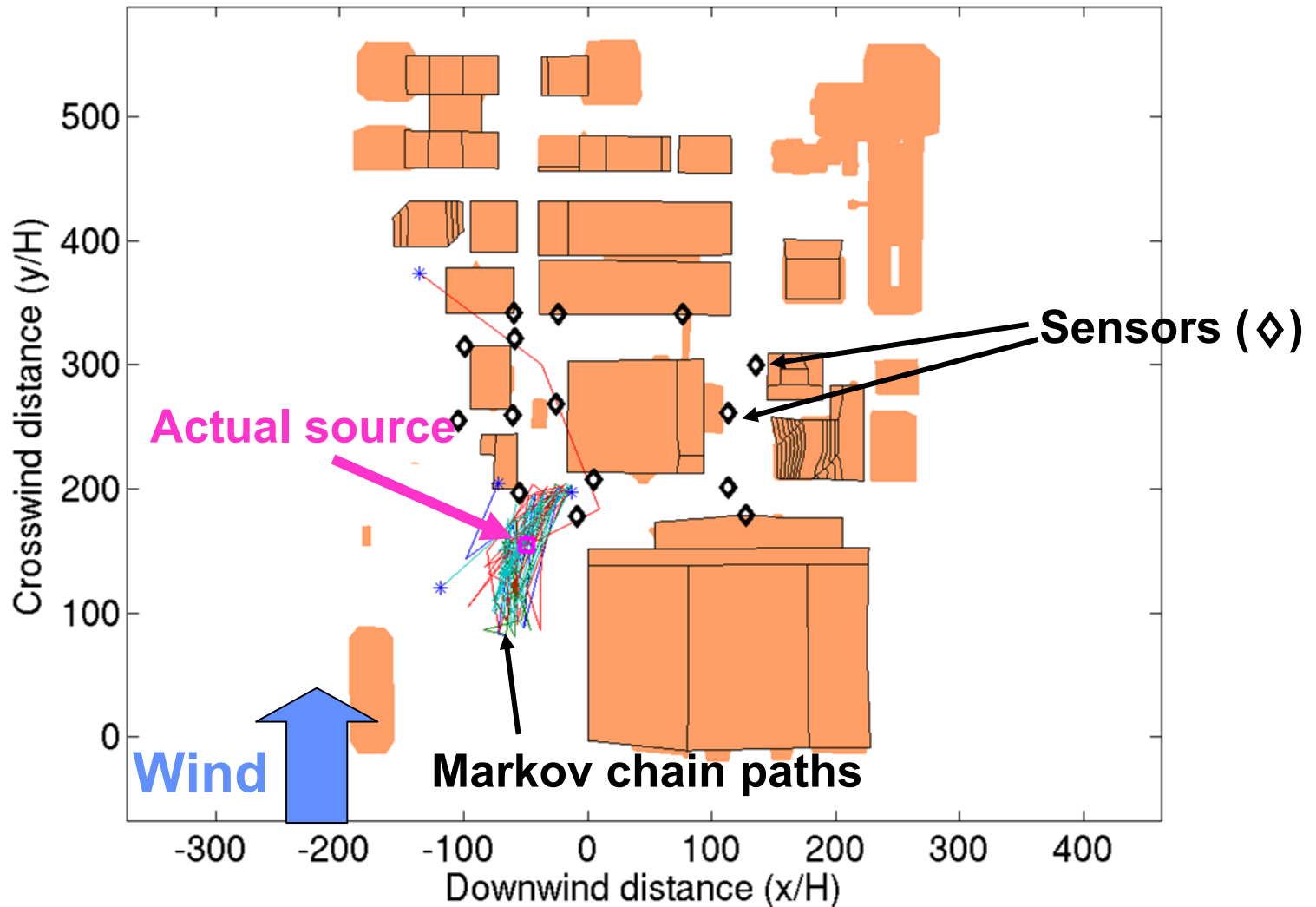


We can exploit computational shortcuts

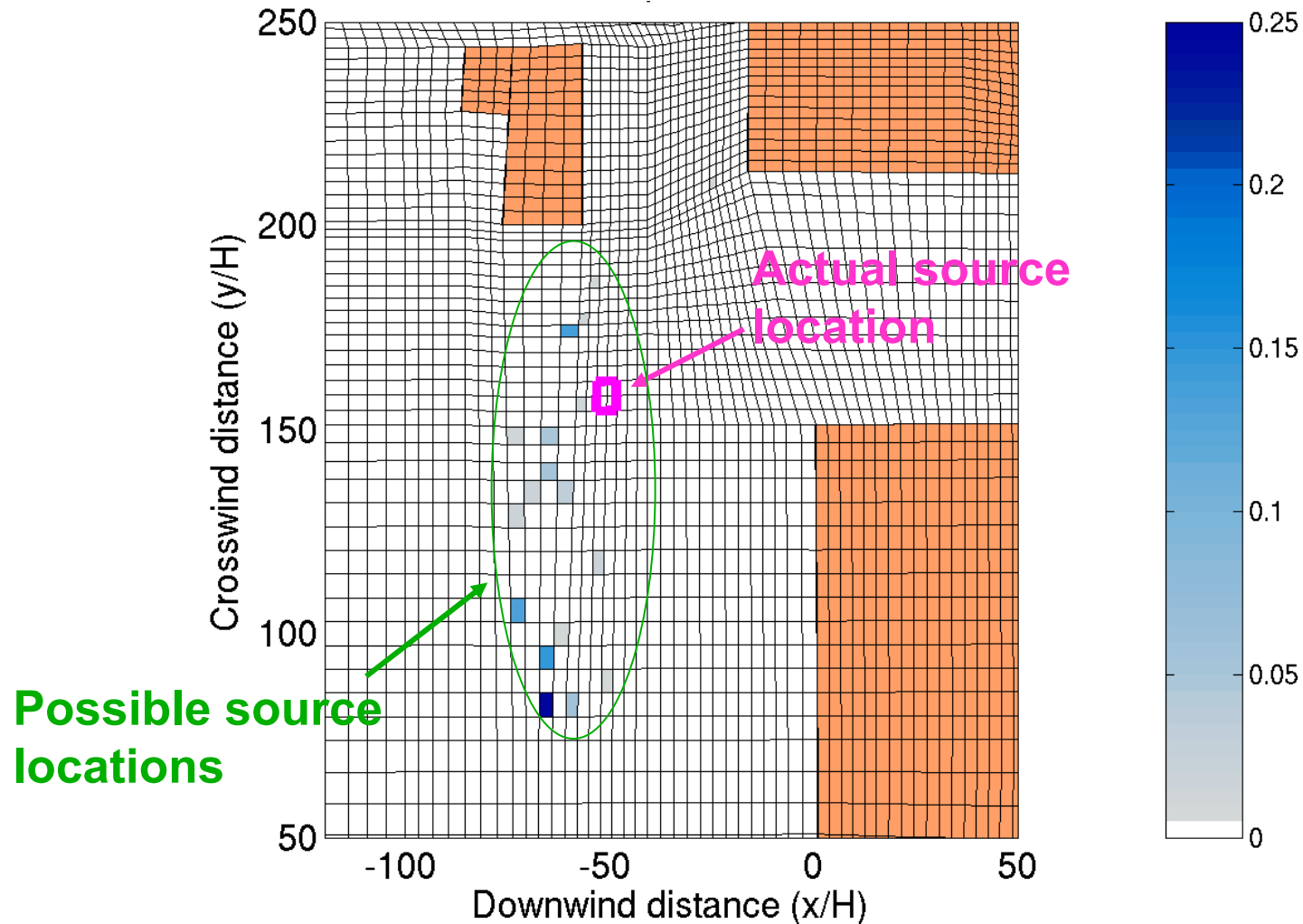
- **Typical inversion requires 20,000 forward runs – too expensive!**
- **Green's function approach**
 - Store runs for unit source at each point in the domain and rescale with sampled source strength
 - Then reconstruction only needs ~2 minutes
- **2560 sources, 128 forward runs required**
 - 20 sources/run using steady wind flow
 - Each forward run uses 32 processors
 - Checkerboard grid to cover larger area
- **Total CPU hours = 13,056**
 - 12+ hours on 1024 2.4 GHz Xeon processors
 - (or 17 days on 32 processors)



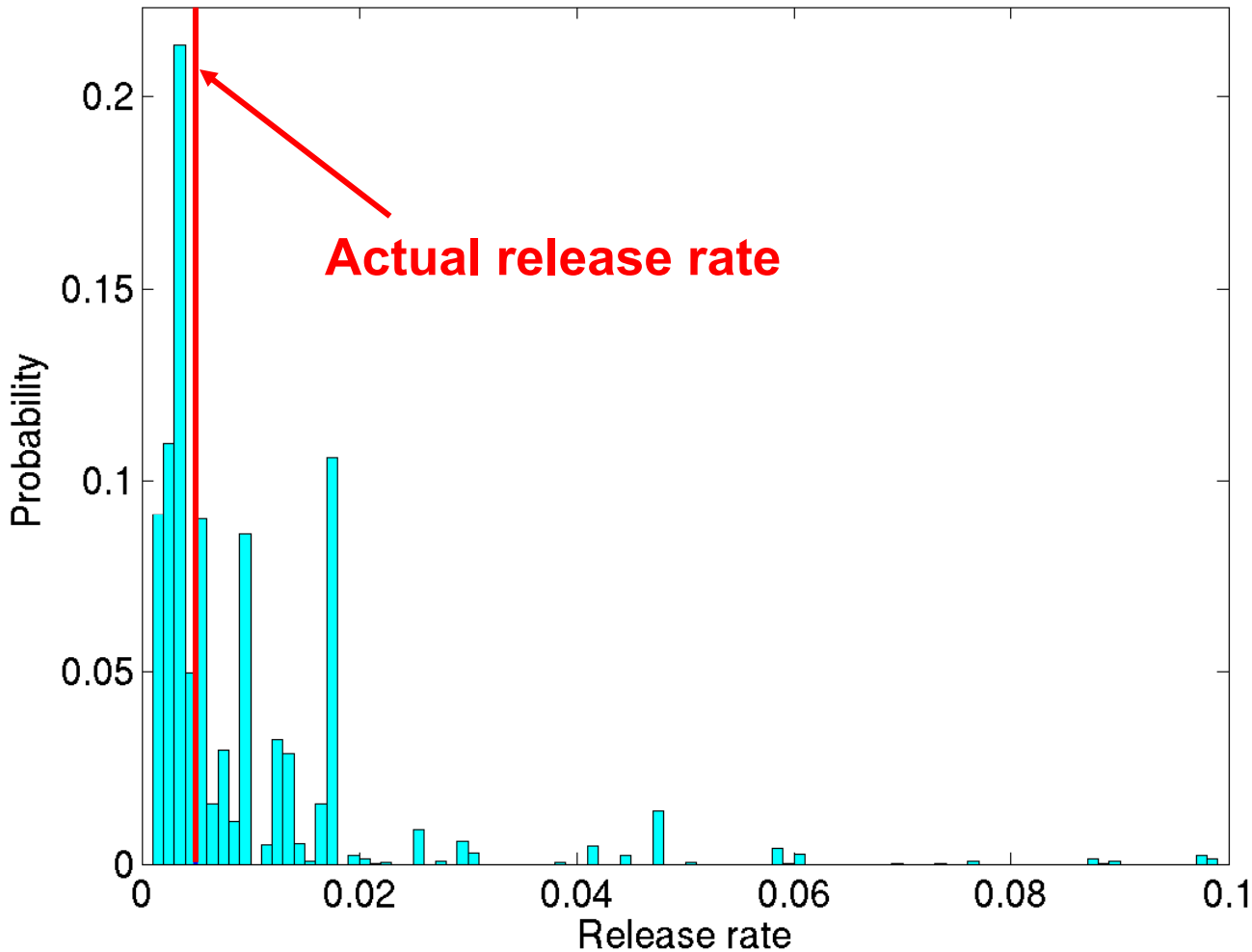
Markov chains quickly focus on source region



Probability distribution of source location estimates likely sources within 100m of actual location



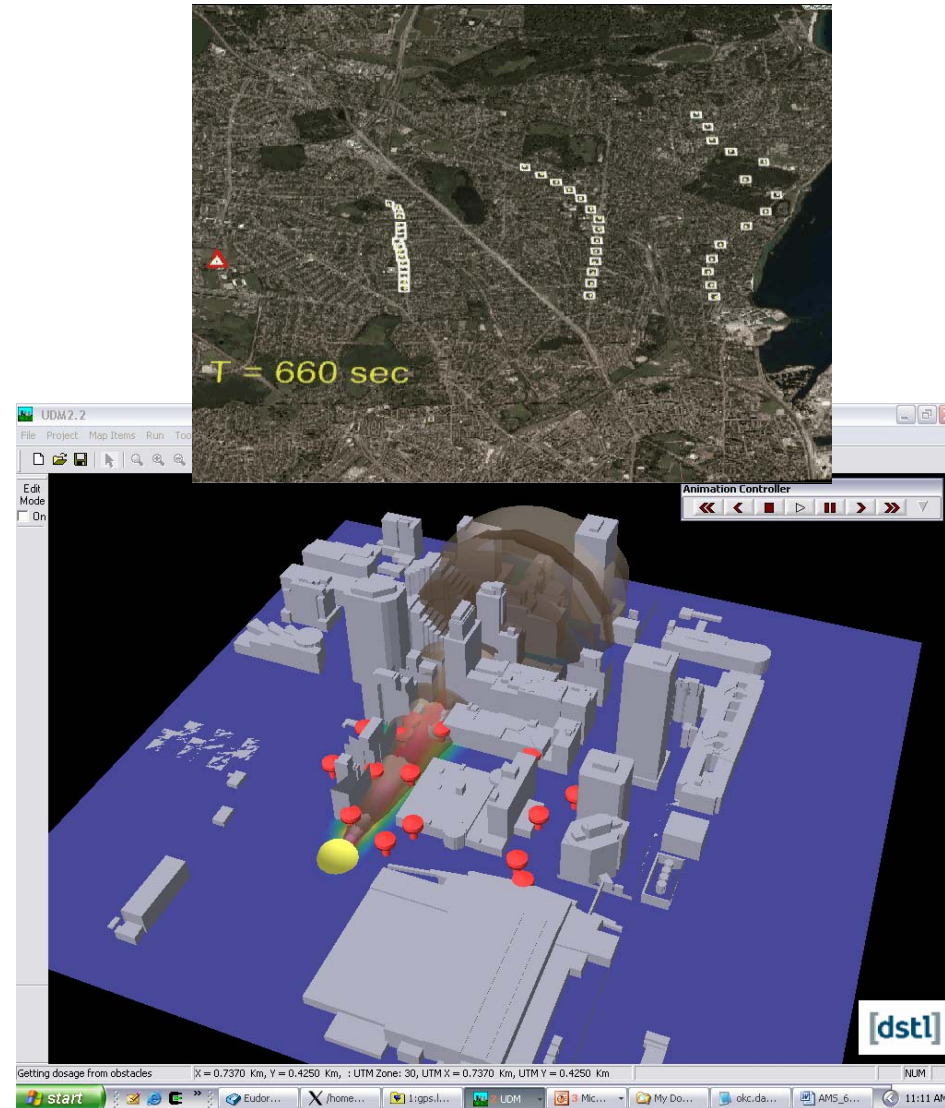
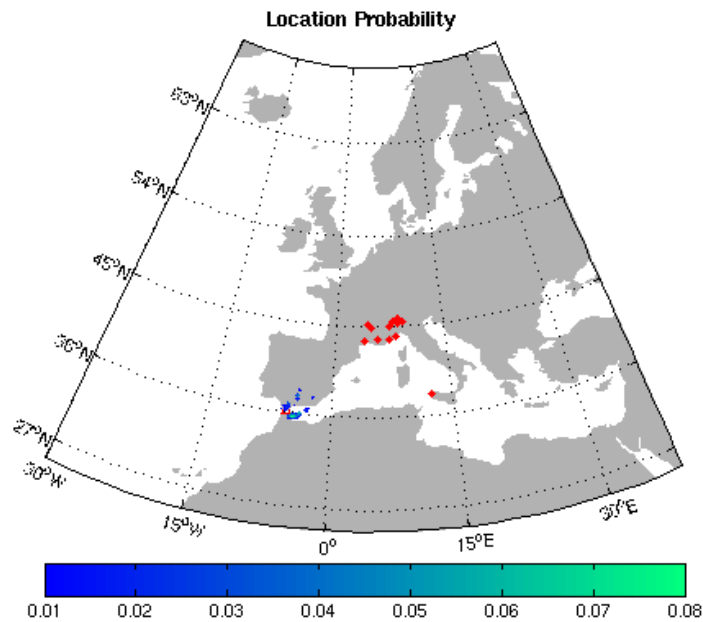
Release rate histogram shows excellent agreement with the actual release rate despite the complexities of the flow



LLNL's Metropolis-Hastings stochastic sampling inversion algorithm is robust and flexible



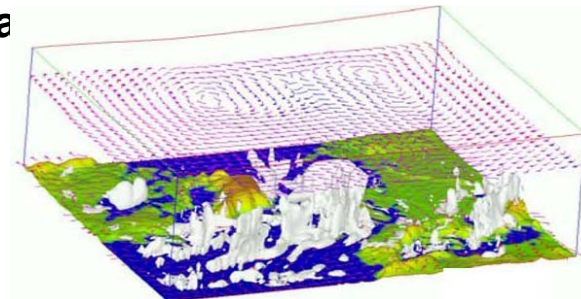
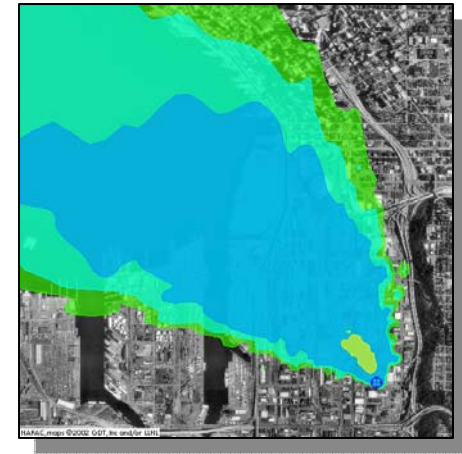
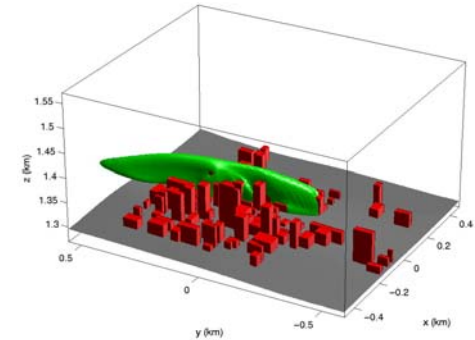
- Multiple scales and types of dispersion problems have been demonstrated and tested:
 - Continental-scale radioactive release
 - Regional scale tracer gas release
 - Urban scale gaseous release (CFD and puff models)



These scientific advances enhance the NARAC Operations Center responses for emergency and routine dispersion simulations



- **FEM3MP simulations inform the development of fast urban parameterizations in NARAC workhorse codes, ADAPT/LODI**
- **FEM3MP runs with mixed/virtual buildings are currently used for planning and exercises**
- **With expanded computational capacity and access to building data sets of more cities, FEM3MP simulations can be used for emergency responses**
 - **Runs currently require 22 hrs of 32 cpus; for one-hour response, 640 processors would be required**
- **Standard WRF can currently provide meteorological information for NARAC's ADAPT/LODI real-time dispersion calculations for emergency response**
- **DRM-WRF, run in-house with expanded computational capacity, would provide improved weather forcing data for NARAC's ADAPT/LODI emergency-response simulations**





Using data from the JU2003 experiment, LLNL scientists have ...

- evaluated and validated our CFD model's performance in the urban core,
- quantified the significant role that advection of turbulence plays in the urban shadow zone,
- defined zone of optimal CFD-performance and zones in which mesoscale effects should be included,
- addressed inadequacies in NWP turbulence modeling and proposed new solutions, now under testing, and
- tested and validated our source reconstruction capability using multiple dispersion models.



Our science team supports customers beyond DOE/DHS

- Design, execution, and analysis of **field campaigns** for verification and validation of NARAC's meteorological and transport/dispersion models
- **Computational Fluid Dynamics** for urban dispersion modeling
- High resolution **numerical weather prediction** (with COAMPS, WRF at 300m resolution) as well as regional climate modeling (at 12 km resolution)
- **Reconstruction** of unknown atmospheric releases from sparse measurements to identify source locations and magnitudes
 - Computational fluid dynamics models in urban areas
 - Simple puff models in urban areas

